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# **Hamiltonian Flow Equations and the Electron-Phonon-Problem**

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**Zusammenfassung** In dieser Arbeit untersuchen wir das Elektron-Phonon-System mit Hilfe von Flussgleichungen für Hamiltonoperatoren. Unter dieser kontinuierlichen Diagonalisierung des Hamiltonoperators werden die Einteilchenenergien und Wechselwirkungskonstanten in Abhängigkeit eines Parameters  $\ell$  transformiert. Dabei variiert  $\ell$  zwischen Null und unendlich. Wir zeigen, dass sich für den Fluss der Einteilchenenergien unter der  $\ell$ -induzierten Transformation asymptotisch für große  $\ell$

$$\epsilon_k(\ell) = \epsilon_k(\infty) + \frac{\text{const}}{2\sqrt{\ell}}$$

ergibt, wobei die Konstante logarithmische Korrekturterme in  $\ell$  enthalten und von  $k$  abhängen kann. Für dieses asymptotische Verhalten wird der Elektron-Phonon-Hamiltonoperator unter der Transformation blockdiagonal. Anschließend zeigen wir, dass sich die Renormierung der Phononen gegenüber den Ergebnissen von Wegner und Lenz nicht verändert, wenn bei diesem Verfahren auch die Verschiebung der elektronischen Einteilchenenergien berücksichtigt wird. Die Abhängigkeit der Renormierung der Elektronen vom Abstand zur Fermikante wird berechnet. Schließlich untersuchen wir die Transformation der elektronischen Einteilchenoperatoren.

Zum Abschluss der Arbeit wird im Anhang ein rigoroser Beweis für das asymptotische Verhalten der Einteilchenenergien gegeben. Es werden logarithmische Korrekturen im asymptotischen Verhalten untersucht.

**Abstract** In this thesis we investigate the electron-phonon-system using the method of Flow Equations for Hamiltonians. In this continuous diagonalisation process the one particle energies and interaction constants are subject to a series of transformations, the “flow” of the Hamiltonian. They depend on a flow parameter  $\ell$  varying from zero to infinity. We give a proof that the asymptotic behaviour of the flow of the one-particle energies for large  $\ell$  is given by:

$$\epsilon_k(\ell) = \epsilon_k(\infty) + \frac{\text{const}}{2\sqrt{\ell}},$$

where the constant may contain terms logarithmic in  $\ell$  and depends on  $k$ . This result is used to show that the transformation does lead to a blockdiagonal Hamiltonian decoupling the electron and the phonon subsystems. We obtain the same renormalization of the phonon energies as Wegner and Lenz, who neglected the shift of the electronic one-particle energies. The dependency of the renormalization of the electronic energies on the distance to the fermi surface is calculated. We investigate the transformation of the electronic one-particle operators.

In the appendix we present a rigorous proof of the asymptotic behaviour. The  $\ell$ -dependency is changed by including an additional logarithmic factor and this refined asymptotic behaviour is investigated.



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# 1. Introduction

There is a wide variety of substances for which at low temperatures the most important interaction is the one between the electrons and the lattice vibrations, which are called phonons. In 1952 Fröhlich [2] proposed a canonical transformation which eliminates the coupling between the phonon and the electron system in first order and instead generates a induced electron-electron interaction. Using the so transformed Hamiltonian Bardeen, Cooper and Schrieffer [3] were able to explain the phenomena of superconductivity in 1956.

Since the discovery of high- $T_c$  superconductivity by Müller/Bednorz [4] in 1986 the correlation of the electron-phonon-interaction with this phenomenon has been discussed and has drawn new attention to the electron-phonon-problem.

Wegner and Lenz [5] investigated the electron-phonon-Hamiltonian using the newly introduced method of Hamiltonian flow equations (Wegner [6]).

The method of flow equations for Hamiltonians is a scheme of a continuous diagonalisation of the Hamiltonian. The one particle energies and interaction constants are subject to a series of transformations depending on a flow parameter  $\ell$ ,  $0 \leq \ell < \infty$ . A short review of this method is given in chapter 2. For  $\ell \rightarrow \infty$  one has to make sure that the off-diagonal interaction vanishes. The change of the one-particle energies under this  $\ell$ -dependent flow then is the renormalization. In general many interaction constants decay rapidly, i.e. exponentially in  $\ell$ . Those remaining decay algebraically. They are responsible for the renormalization of the one-particle energies.

Wegner and Lenz applied the formalism of Hamiltonian flow equations to the electron-phonon-problem such that the Hamiltonian is only brought to a block-diagonal form. Besides the renormalization of the one-particle energies the difference of the diagonalized Hamiltonian to a system of free electrons and phonons is an attractive electron-electron interaction. For the flow of the energies and interaction constants under the series of  $\ell$ -dependent transformations Wegner and Lenz found a fundamental set of integro-differential equations. This set is the basis of this thesis.

Neglecting any renormalization for the electron energies Wegner and Lenz investigated the renormalization of the phononic energies and they obtained an improved attractive mediate electron-electron interaction. Continuing this work Wegner and Ragwitz [7] calculated the renormalization of the phonon energies and the correlation functions of the phonons. Once again the electronic energies were taken as constants under the diagonalisation of the electron-phonon-Hamiltonian.

In this thesis we will follow the lines of their work but include the renormalization of the electronic one particle energies. The result is twofold:

First, we are able to show that the renormalization of the phonons is not changed when the renormalization of the electrons is included.

Second, we can justify that the renormalization of the electrons due to this transformation is small compared to the effects of the attractive electron-electron-interaction.

The organisation of this thesis is as follows:

In chapter 2 we give a more detailed introduction to the formalism of flow-equations for Hamiltonians as introduced by Wegner [6] in 1993.

In chapter 3 we introduce the electron-phonon-problem and give a derivation of the equations for the renormalization of this system as obtained by Wegner and Lenz [5]. We also give a short overview of the results they found in their paper for the attractive electron-electron interaction.

We find in chapter 4 the general behaviour of the asymptotic form (in  $\ell$ ) of the electron and the phonon energies. A rigorous proof for this solution is given in appendix A. We also show in chapter 4 that indeed the electron-phonon interaction vanishes as the series of transformations proceed with increasing  $\ell$ . A solution of the fundamental set of equations is found in the following self consistent way: First certain functions of the parameter  $\ell$  for the electron and phonon energies are assumed and then it is proved that the fundamental equations are fulfilled.

In chapter 5 we look for a solution using a more refined dependence on  $\ell$  for smaller  $\ell$ -values. In this ansatz we specify some details to reach a fully self-consistent solution in chapter 6.

The transformation of the electronic one-particle operators under the  $\ell$  induced flow is investigated in chapter 7.

The results of the thesis, including a different approach for the exact asymptotic behaviour as given in Appendix B, are discussed in chapter 8.

## 2. Flow Equations for Hamiltonians

### 2.1. Transformation of the Hamiltonian

Every quantummechanical system is characterized by a Hamiltonian. The eigenvalues of this hermitian operator give the energy levels of the system, the corresponding eigenvectors describe the allowed states. Hence, to investigate a physical system in quantum mechanics one tries to diagonalize the corresponding Hamiltonian,i.e. one searches for a unitarian operator  $U$  such that

$$U^+ H U = D \quad (2.1)$$

where  $D$  has diagonal form.

However, for most systems physics is interested in such a unitarian transformation cannot be given explicitly. Instead approximation schemes have to be used.

A new method to reach a diagonal Hamiltonian was proposed by Franz Wegner in 1993. One writes an ensemble of transformations characterized by a parameter  $\ell$ ,  $0 < \ell < \infty$

$$H(\ell) = U^+(\ell) H_0 U(\ell) \quad U(0) = 1 \quad (2.2)$$

Here  $H_0$  is the Hamiltonian describing the entire system. The subindex 0 is only used to denote  $H_0$  as the starting point of the  $\ell$ -dependent transformation.  $H_0$  is not diagonal. At the start,  $\ell = 0$ , a basis is chosen which represents the actual physical system in an approximate way. These approximate states are then transformed by  $U^+(\ell)$ .

In this approach the Hamiltonian is not diagonalized in one step but for every given  $\ell_0$  one tries to find a change  $dH(\ell_0)$  such that  $H(\ell_0 + d\ell)$  has smaller off-diagonal terms than  $H(\ell_0)$ . The infinitesimal change of  $H(\ell)$  is given by:

$$\frac{dH(\ell)}{d\ell} = [\eta(\ell), H(\ell)] \quad (2.3)$$

where  $\eta(\ell) = \frac{dU^+(\ell)}{d\ell} U(\ell)$  is antihermitian. Except for this condition the choice of  $\eta$  is free. The ensemble of antihermitian matrices is chosen such that  $H(\ell = \infty)$  has diagonal or at least blockdiagonal form and the resulting differential equations for the

“flow” of the elements  $h_{i,j}(\ell)$  of  $H(\ell)$  as a function of  $\ell$  take a form as simple as possible. Wegner proposed:

$$\eta(\ell) = [H_d(\ell), H_r(\ell)] \quad (2.4)$$

as a possible choice for  $\eta$ .  $H_d$  and  $H_r$  are the diagonal and offdiagonal terms of the Hamiltonian, respectively. The hope is that  $H_r(\ell) \rightarrow 0$  as  $\ell \rightarrow \infty$  for such an  $\eta$ . Unfortunately this is not generally true, even if  $\eta$  vanishes with  $\ell$  tending to infinity! Therefore, when applying an  $\eta$  of the form of (2.4) it has to be investigated for each physical system whether or not  $H_r$  does indeed vanish.

Transforming a Hamiltonian within the framework of this formalism of Flow-equations will, in general, generate terms not present in the original Hamiltonian. In some exceptional cases it is possible to include all the additional terms in the formalism. Otherwise, the additional terms can only be treated approximately. The approximations depend, of course, on the physical system, the corresponding Hamiltonian, the physical quantities under considerations and the form of the additional terms. The goal is always to keep the error as small as possible.

The result of the procedure sketched above is a set of coupled differential equations governing the flow of the self-energy of the particles and the interaction constants as a function of the parameter  $\ell$  where the interaction constants vanish as  $\ell \rightarrow \infty$ .

## 2.2. Transformation of physical quantities

Actually the Hamiltonian itself does not change under the  $\ell$  dependent transformation; for every  $\ell$  the Hamiltonian is represented in a different basis and the change of the basis is given by the ensemble of the unitarian transformations. This has to be kept in mind, if one is interested in physical properties of the quantummechanical system under investigation. Lets take the expectation value of a hermitian operator  $O$ . Then we have to take  $O$  in its transformed representation:

$$O(\ell) = U^+(\ell)OU(\ell) \quad (2.5)$$

In the limit for which our Hamiltonian is (block-)diagonal, this reads:

$$\langle O(\infty) \rangle = \langle U^+(\infty)OU(\infty) \rangle \quad (2.6)$$

In general we do not know  $U(\infty)$  and have to find  $O(\infty)$  by once again applying the flow equation formalism with the same  $\eta$  as used for the transformation of the Hamiltonian:

$$\frac{dO(\ell)}{d\ell} = [\eta(\ell), O(\ell)] \quad (2.7)$$

## 3. The Electron-Phonon-Problem

### 3.1. The Hamiltonian

The Hamiltonian of the electron-phonon problem is given by:

$$H_0 = \sum_k \epsilon_k c_k^\dagger c_k + \sum_q \omega_q a_q^\dagger a_q + \sum_{k,q} M_q (a_{-q}^\dagger + a_q) c_{k+q}^\dagger c_k \quad (3.1)$$

Further interactions (e.g. coulomb-interaction) and higher order terms are neglected. For reasons of simplification we work with electrons of one band only.

The first term of (3.1) is the self-energy term of the free electrons.

The second term describes “free” phonons. These characterize the vibrations of the ions of the lattice. The third term is the electron-phonon-interaction discussed in 3.1.2.

#### 3.1.1. Phonons

The ions of the lattice oscillate around their equilibrium positions<sup>1</sup>. This leads to vibrations of the lattice for which the (classical) hamiltonian function is given (up to second order) by:

$$H = \sum_{n,i} \frac{M}{2} \dot{s}_{n,i}^2 + \frac{1}{2} \sum_{\substack{n,i \\ n',i'}} \frac{\partial^2 V}{\partial R_{n,i} \partial R_{n',i'}} s_{n,i} s_{n',i'} \quad (3.2)$$

$s_{n,i}$  is the  $i$ th cartesian coordinate of the displacement of the ions of the  $n$ th Wigner-Seitz cell.  $V$  is the potential in which the ions move.

We put:

$$\begin{aligned} s_{n,i} &= \frac{1}{\sqrt{M}} u_{n,i} e^{-i\omega t}, \\ u_{n,i} &= c_i e^{i\mathbf{q}\mathbf{R}_n}, \text{ and} \\ D_{n,i}^{n',i'} &= \frac{1}{M} \frac{\partial^2 V}{\partial R_{n,i} \partial R_{n',i'}}; \end{aligned}$$

the equation of motion then yields:

$$\omega^2 c_i = \sum_{i'} \left\{ \sum_{n'} D_{n,i}^{n',i'} \exp[i\mathbf{q}(\mathbf{R}_{n'} - \mathbf{R}_n)] \right\} c_{i'}. \quad (3.3)$$

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<sup>1</sup>For a more detailed introduction of phonons see: [1]

The translational symmetry requires that  $D_{n,i}^{n',i'}$  does not depend on the cell indices  $n$  and  $n'$  separately, but can only depend on  $(n - n')$ . The solution of (3.3) is given by three different eigenvalues  $\omega^{(j)}$ , which depend on  $\mathbf{q}$ . For each  $\omega^{(j)}(\mathbf{q})$  the components of the corresponding eigenvector are given by:  $c_i = e_i^{(j)}(\mathbf{q})$ . These solutions form vectors  $\mathbf{e}^{(j)}(\mathbf{q})$ , which are orthonormal. As a set of special solutions for the displacements  $\mathbf{s}_n(t)$  it is possible to use:

$$\mathbf{s}_n^{(j)}(\mathbf{q}, t) = \frac{1}{\sqrt{M}} \mathbf{e}^{(j)}(\mathbf{q}) \exp(i[\mathbf{q}\mathbf{R}_n - \omega_j(\mathbf{q})t]). \quad (3.4)$$

The general solutions can be constructed by superposition of the special ones:

$$\mathbf{s}_n(\mathbf{q}, t) = \frac{1}{\sqrt{NM}} \sum_{j,\mathbf{q}} Q_j(\mathbf{q}, t) \mathbf{e}^{(j)}(\mathbf{q}) \exp(i\mathbf{q}\mathbf{R}_n) \quad (3.5)$$

the time dependency has been included in the factor  $Q_j(\mathbf{q}, t)$  a factor  $\frac{1}{\sqrt{N}}$  has been separated out. In the usual way (3.2) can be quantized and written as:

$$H = \frac{1}{2} \sum_{j,\mathbf{q}} [\dot{Q}_j^*(\mathbf{q}, t) \dot{Q}_j(\mathbf{q}, t) + \omega_j^2 Q_j^*(\mathbf{q}, t) Q_j(\mathbf{q}, t)]. \quad (3.6)$$

With the usual transformation (as applied for the harmonic oscillator):

$$\begin{aligned} P_j(\mathbf{q}, t) &= \dot{Q}_j(\mathbf{q}, t), \\ a_q &= (2\hbar\omega(\mathbf{q}))^{-\frac{1}{2}} (\omega(\mathbf{q})Q_j(\mathbf{q}) + iP^*(\mathbf{q})) \text{ and} \\ a_q^\dagger &= (2\hbar\omega(\mathbf{q}))^{-\frac{1}{2}} (\omega(\mathbf{q})Q_j^*(\mathbf{q}) - iP(\mathbf{q})) \end{aligned}$$

we then find the Hamiltonian for the free *phonons*:

$$H = \sum_{j,\mathbf{q}} \hbar\omega_j(\mathbf{q}) \left[ a_j^\dagger(\mathbf{q}) a_j(\mathbf{q}) + \frac{1}{2} \right] \quad (3.7)$$

### 3.1.2. The electron-phonon-interaction

In this section a short derivation of the interaction electron-phonon-interaction is given<sup>2</sup>.

In general the interaction of electrons and ions is given by:

$$H_{el-ion} = \sum_{l,n} V_{el-ion}(r_l - R_n) \quad (3.8)$$

Here we use Nordheim's rigid ion model in which the interaction depends only on the separation of electrons and ions; the form of the ions does not change during the motion.

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<sup>2</sup>We closely follow [1] where a more detailed analysis is given

Most of the more sophisticated models do not alter the electron-phonon interaction in a significant way. Therefore, the results of this thesis do not depend on the choice of the specific model.

Let the position of an ion be given by:  $\mathbf{R}_n + \mathbf{s}_n$ .  $\mathbf{R}_n$  denotes the equilibrium position of the  $n$ th ion and  $\mathbf{s}_n(t)$  its displacement from this position. As  $\mathbf{s}_n$  is small compared to the size of a unit cell we can expand (3.8) to find:

$$H_{el-ion} = \sum_{l,n} V_{el-ion}(\mathbf{r}_l - \mathbf{R}_n) + \sum_{l,n} \vec{\nabla} V_{el-ion}(\mathbf{r}_l - \mathbf{R}_n) \cdot \mathbf{s}_n \quad (3.9)$$

$$= H_{el-ion}^0 + H_{el-ph}. \quad (3.10)$$

The first term describes the interaction of the electrons with the periodic potential of the ionic background. In this subsection we are interested in the second term which is the electron-phonon interaction coupling the electrons and the lattice vibrations. Using normal coordinates for  $\mathbf{s}_n$  gives:

$$H_{el-ph} = \sum_{n,l} \frac{1}{\sqrt{NM}} \sum_{\mathbf{q},j} Q_{\mathbf{q},j} \exp(i\mathbf{q} \cdot \mathbf{R}_n) e^j(\mathbf{q}) \cdot \vec{\nabla} V_{el-ion}(\mathbf{r}_l - \mathbf{R}_n). \quad (3.11)$$

For every normal coordinate the phonon component

$$Q_{\mathbf{q}} = \left( \frac{\hbar}{2\omega_{\mathbf{q},j}} \right) (a_{-\mathbf{q},j}^\dagger + a_{\mathbf{q},j})$$

consists of two parts: One creating a phonon with (pseudo)momentum  $-\mathbf{q}$  and one absorbing a phonon with pseudomomentum  $\mathbf{q}$ . This (pseudo)-momentum has to be delivered by the electrons. We expand  $\vec{\nabla} V$  in  $k$ -space (N.B. The interaction potential does not depend on the spins):

$$\begin{aligned} \vec{\nabla} V &= \sum_{\mathbf{k}, \mathbf{k}', \sigma} \langle \mathbf{k}' \sigma | \vec{\nabla} V | \mathbf{k} \sigma \rangle c_{\mathbf{k}', \sigma}^\dagger c_{\mathbf{k}, \sigma} \\ &= \sum_{\mathbf{k}, \mathbf{k}', \sigma, \boldsymbol{\kappa}} \exp(-i\boldsymbol{\kappa} \cdot \mathbf{R}_n) V_{\boldsymbol{\kappa}} \langle \mathbf{k}' \sigma | \exp(-i\boldsymbol{\kappa} \cdot \mathbf{r}) | \mathbf{k} \sigma \rangle c_{\mathbf{k}', \sigma}^\dagger c_{\mathbf{k}, \sigma}. \end{aligned} \quad (3.12)$$

The electrons are described by Bloch functions:  $|\mathbf{k}\rangle = u_n(\mathbf{k}, \mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}$ . We use  $\sum_n \exp[i(\mathbf{q} - \boldsymbol{\kappa}) \cdot \mathbf{R}_n] = N \sum_{\mathbf{K}_m} \delta_{\mathbf{q}, \boldsymbol{\kappa} + \mathbf{K}_m}$ . Here  $\mathbf{K}_m \cdot \mathbf{R}_n$  is a multiple of  $2\pi$  for all  $n$ . Terms with  $\mathbf{K}_m \neq 0$  describe Umklapp-processes.

As we are interested in the behaviour of the system at low temperatures, i.e. only phonon-levels with small  $q$  are occupied, we restrict our considerations to normal processes, i.e.  $\mathbf{K}_m = 0$ .

$$\begin{aligned}
H_{el-ph} &= \sum_{\mathbf{k}, \sigma, j, \mathbf{q}} \sqrt{\frac{N}{M}} V_{\kappa} i \mathbf{q} \cdot \mathbf{e}^j(\mathbf{q}) \sqrt{\frac{\hbar}{2\omega_{\mathbf{q},j}}} \\
&\times \int u_n^*(\mathbf{k} + \mathbf{q}, \mathbf{r}) u_n(\mathbf{k}, \mathbf{r}) d\mathbf{r} (a_{-\mathbf{q},j}^\dagger + a_{\mathbf{q},j}) c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{\mathbf{k},\sigma}.
\end{aligned} \tag{3.13}$$

We further use a phonon representation which is either purely longitudinal or purely transverse, i.e. the oscillations are parallel or perpendicular to  $\mathbf{q}$ . Then only the longitudinal phonons couple to the electrons. Finally we obtain:

$$H_{el-ph} = \sum_{\mathbf{k}, \sigma, \mathbf{q}} M_{\mathbf{k}\mathbf{q}} (a_{-\mathbf{q}}^\dagger + a_{\mathbf{q}}) c_{\mathbf{k}+\mathbf{q},\sigma}^\dagger c_{\mathbf{k},\sigma} \tag{3.14}$$

with:  $M_{k,q} = iV_{\mathbf{q}}q \sqrt{\frac{N}{M}} \sqrt{\frac{\hbar}{2\omega_{\mathbf{q}}}} \int u_n^*(\mathbf{k} + \mathbf{q}, \mathbf{r}) u_n(\mathbf{k}, \mathbf{r}) d\mathbf{r}$

For nearly free electrons the integral is approximately one, yielding:

$$M_q = iV_{\mathbf{q}}q \sqrt{\frac{N}{M}} \sqrt{\frac{\hbar}{2\omega_{\mathbf{q}}}} \tag{3.15}$$

This gives the interaction term of (3.1).

### 3.2. Applying the Flow Equations to the Electron-Phonon-Problem

Wegner and Lenz applied the formalism of Flow Equations to the electron-phonon Hamiltonian (3.1) [5].

They used the following  $\eta$ :

$$\begin{aligned}
\eta(\ell) &= \\
&\left[ \sum_q \omega_q(\ell) : a_q^+ a_q : + \sum_k \epsilon_k(\ell) : c_k^+ c_k : , \sum_{k,q} (M_{k,q}(\ell) a_{-q}^+ + M_{k+q,-q}(\ell) a_q) c_{k+q}^+ c_k \right] \\
&= \sum_{k,q} (\alpha_{k,q}(\ell) M_{k,q}(\ell) a_{-q}^+ - \alpha_{k+q,-q}(\ell) M_{k+q,-q}(\ell) a_q) c_{k+q}^+ c_k
\end{aligned} \tag{3.16}$$

with:

$$\alpha_{k,q} = \epsilon_{k+q} - \epsilon_k + \omega_q.$$

This gives the energy which is needed for or gained by one interaction process. It is the change of energy of the electron changing its momentum plus the energy put into the creation of a phonon or gained by its annihilation.

This is the choice of  $\eta$  proposed by Wegner (2.4).



Here  $\sum_q \omega_q(\ell) : a_q^\dagger a_q : + \sum_k \epsilon_k(\ell) : c_k^\dagger c_k :$  is the diagonal and

$\sum_{k,q} (M_{k,q}(\ell) a_{-q}^\dagger + M_{k+q,-q}(\ell) a_q) c_{k+q}^\dagger c_k$  is the off-diagonal part of the Hamiltonian.

We will show later 4.4 that for this choice of  $\eta$  the interaction constants  $M_{k,q}$  do indeed vanish for  $\ell \rightarrow \infty$ .

During the transformation process the Hamiltonian is given by:

$$\begin{aligned} H(\ell) = & \sum_q \omega_q(\ell) : a_q^\dagger a_q : + \sum_k \epsilon_k(\ell) : c_k^\dagger c_k : \\ & + \sum_{k,k',q} V_{k,k',q}(\ell) : c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k : + E(\ell) \\ & + \sum_{k,q} (M_{k,q}(\ell) a_{-q}^\dagger + M_{k+q,-q}(\ell) a_q) c_{k+q}^\dagger c_k \end{aligned} \quad (3.17)$$

with the initial values:

$$\begin{aligned} M_{k,q}(\ell=0) = M_{k+q,-q}(\ell=0) = M_q(0) = M_q = \tilde{c}\sqrt{q} \\ V_{k,k',q}(\ell=0) = 0 \\ \omega_q(\ell=0) = \tilde{c}|q| \quad \epsilon_k(\ell=0) = \frac{k^2}{2m} \end{aligned} \quad (3.18)$$

These values are those on a lattice with a periodicity length  $a$  of e.g. cubic form:  $\epsilon_{k+2\pi a} = \epsilon_k$ . The interaction constant  $\tilde{c}$  contains a factor  $\frac{1}{\sqrt{N}}$ . An additional electron-electron-interaction is generated during the transformation process. This interaction is attractive and eventually leads to superconductivity<sup>3</sup>.

Actually, during the transformation more terms than given above are generated. These additional terms are of higher order, e.g. four particle interactions. It makes some sense not to keep terms which have originally been considered to be unimportant for our investigation.

In order to neglect these additional terms and still keep the error in the calculation as small as possible the Hamiltonian is rewritten in its normal ordered form. Then the expectation value of the neglected terms with respect to the canonical ensemble is zero. Changing the Hamiltonian to its normal ordered form yields  $E(\ell)$ , the ground state expectation value of the energy<sup>4</sup>. In the following we will mostly work in the regime of zero temperature. The expectation values are consequently taken with respect to the ground state.

For  $\ell \rightarrow \infty$  we expect to find:

$$H(\infty) = \sum_q \omega_q(\infty) : a_q^\dagger a_q : + \sum_k \epsilon_k(\infty) : c_k^\dagger c_k :$$

<sup>3</sup>See [5]

<sup>4</sup>Some of the additional terms which would be generated during the transformation can be gotten rid of by adding small terms to  $\eta$ . For a more detailed analysis see [5].

$$+ \sum_{k,k',q} V_{k,k',q}(\infty) : c_{k+q}^+ c_{k'-q}^+ c_{k'} c_k : + E(\infty).$$

The flow of the terms in (3.17) is governed by the following set of coupled differential equations<sup>5</sup>:

$$\begin{aligned} \frac{dM_{k,q}}{d\ell} &= -\alpha_{k,q}^2 M_{k,q} \\ \frac{d\omega_q}{d\ell} &= 2 \sum_k |M_{k,q}|^2 \alpha_{k,q} (n_{k+q} - n_k) \\ \frac{d\epsilon_k}{d\ell} &= -2 \sum_q |M_{k,q}|^2 \alpha_{k,q} (1 - n_{k+q} + n_q) \\ &\quad + 2 \sum_q |M_{k+q,-q}|^2 \alpha_{k+q,-q} (n_{k+q} + n_q) \\ \frac{dV_{k,k',q}}{d\ell} &= -M_{k,q} M_{k'-q,q} \alpha_{k'-q,q} - M_{k+q,-q} M_{k',-q} \alpha_{k',-q} \\ \frac{dE}{d\ell} &= \sum_{k,q} n_{k+q} (|M_{k,q}|^2 \alpha_{k,q} - |M_{k+q,-q}|^2 \alpha_{k+q,-q}) \end{aligned} \tag{3.19}$$

The  $n_k$  and  $n_q$  are the occupation numbers of the electronic and phononic states, respectively. To find these equations one simply compares the coefficients of the operators in:

$$\begin{aligned} \frac{dH(\ell)}{d\ell} &= [\eta(\ell), H(\ell)] \\ \sum_q \frac{d\omega_q(\ell)}{d\ell} : a_q^+ a_q : \dots &= 2 \sum_k |M_{k,q}|^2 \alpha_{k,q} (n_{k+q} - n_k) : a_q^+ a_q : \dots \end{aligned} \tag{3.20}$$

For  $T = 0$  the  $n_q$  equal zero as the expectation value to find a phonon is 0.

In the subsequent chapters we will use this set of coupled differential equations for  $T = 0$  to investigate the asymptotic behaviour of the one particle energies and the interaction constants and thus calculate their ongoing renormalization as  $\ell$  increases.

### 3.2.1. Results of Wegner and Lenz for this set of equations

Wegner and Lenz used the equations (3.19) to investigate the attractive electron-electron-interaction and the flow of the phononic energies. Their result for the induced electron-electron interaction is an improvement as compared to the one found by Fröhlich [2]. These expressions are noted here.

The interaction for cooper pairs as found by Fröhlich is:

$$V_{k,-k,q} = |M_q|^2 \frac{\omega_q}{(\epsilon_{k+q} - \epsilon_k)^2 - \omega_q^2} \tag{3.21}$$

---

<sup>5</sup>The equations as given above are a simplification made by Wegner and Lenz. Only terms up to second order in the interaction constant are kept [5].

whereas Wegner and Lenz found:

$$V_{k,-k,q} = -|M_q|^2 \frac{\omega_q}{(\epsilon_{k+q} - \epsilon_k)^2 + \omega_q^2}. \quad (3.22)$$

In (3.21) there is a singularity and for  $(\epsilon_{k+q} - \epsilon_k)^2 > \omega_q^2$  the interaction is repulsive. The interaction (3.22) is attractive for all Cooper pairs and no singularity exists. For a more detailed analysis see [5].



## 4. The General Asymptotic Behaviour

### 4.1. General Transformations

As a starting point for the search of the asymptotic behaviour consider the equations (3.19) for  $T = 0$  (i.e.  $n_q = 0$ ):

$$\frac{dM_{k,q}(\ell)}{d\ell} = -\alpha_{k,q}^2(\ell)M_{k,q}(\ell) \quad (4.1)$$

$$\frac{d\omega_q(\ell)}{d\ell} = 2 \sum_k |M_{k,q}|^2 \alpha_{k,q}(n_{k+q} - n_k) \quad (4.2)$$

$$\frac{d\epsilon_k(\ell)}{d\ell} = -2 \sum_q |M_{k,q}|^2 \alpha_{k,q}(1 - n_{k+q}) \quad (4.3)$$

$$+ 2 \sum_q |M_{k+q,-q}|^2 \alpha_{k+q,-q} n_{k+q} \quad (4.4)$$

$$\frac{dV_{k,k',q}(\ell)}{d\ell} = -M_{k,q} M_{k'-q,q} \alpha_{k'-q,q} - M_{k+q,-q} M_{k',-q} \alpha_{k',-q} \quad (4.5)$$

once again  $\alpha_{k,q} = \epsilon_{k+q} - \epsilon_k + \omega_q$ . The initial values are given by (3.18).

In the infinite volume limit these equations can be written in integral form:

$$\frac{dM_{k,q}(\ell)}{d\ell} = -\alpha_{k,q}^2(\ell)M_{k,q}(\ell) \quad (4.6)$$

$$\frac{d\omega_q(\ell)}{d\ell} = 2 \frac{V}{(2\pi)^3} \int_B d^3k |M_{k,q}|^2 \alpha_{k,q}(n_{k+q} - n_k) \quad (4.7)$$

$$\frac{d\epsilon_k(\ell)}{d\ell} = -2 \frac{V}{(2\pi)^3} \int_B d^3q |M_{k,q}|^2 \alpha_{k,q}(1 - n_{k+q}) \quad (4.8)$$

$$+2\frac{V}{(2\pi)^3}\int_B d^3q|M_{k+q,-q}|^2\alpha_{k+q,-q}n_{k+q} \quad (4.9)$$

$$\frac{dV_{k,k',q}}{d\ell} = -M_{k,q}M_{k'-q,q}\alpha_{k'-q,q} - M_{k+q,-q}M_{k',-q}\alpha_{k',-q}. \quad (4.10)$$

$B$  is the first Brillouin-Zone; we use  $\epsilon(k+q) = \frac{(k+q)^2}{2m}$  even for  $(k+q)$  outside the first Brillouin zone as we will be interested only in the vicinity of the Fermi surface. As

$$T=0 \text{ } n_k \text{ is given by: } n_k = \begin{cases} 1 & |k| < k_f \\ 0 & k > k_f \end{cases}$$

We can integrate (4.6) formally:

$$M_{k,q}(\ell) = M_q e^{-\int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \quad (4.11)$$

Using this expression the derivatives of  $\omega_q(\ell)$  and  $\epsilon_k(\ell)$  can be written as:

$$\frac{d\omega_q(\ell)}{d\ell} = 2\Gamma \int_B d^3k \alpha_{k,q}(\ell) |M_q|^2 e^{-2\int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} (n_{k+q} - n_k) \quad (4.12)$$

$$\frac{d\epsilon_k(\ell)}{d\ell} = -2\Gamma \int_B d^3q \alpha_{k,q}(\ell) |M_q|^2 e^{-2\int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} (1 - n_{k+q}) \quad (4.13)$$

$$+2\Gamma \int_B d^3q \alpha_{k+q,-q}(\ell) |M_q|^2 e^{-2\int_0^\ell \alpha_{k+q,-q}^2(\ell') d\ell'} n_{k+q} \quad (4.14)$$

$$\Gamma := \frac{V}{(2\pi)^3}.$$

## 4.2. Establishing a $\frac{1}{\sqrt{\ell}}$ behaviour

To investigate the equations above we first take a look at the integral:

$$\int_B d^3q \alpha_{k,q}(\ell) |M_q|^2 e^{-2\int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \quad (4.15)$$

The integral  $\int d^3k \alpha_{k,q}(\ell) |M_q|^2 e^{-2\int_0^\ell \alpha_{k,q}^2(\ell') d\ell'}$  determining the derivative of  $\omega_q$  is treated in exactly the same way. Hence, we will present the details for the integral (4.15) only. For a more detailed analysis and the analysis of the integral  $\int d^3k \dots$  see appendix A. Our aim is to find a self consistent solution of (4.12) and (4.13) for large  $\ell$ . We assume the asymptotic form of the  $\epsilon_k(\ell)$  and  $\omega_q(\ell)$  contained in  $\alpha$  which we use to find the asymptotic behaviour of an integral of the form (4.15). The integral is then used to calculate the behaviour of the one particle energies according to equations (4.12),

(4.13). This has to be in accordance with the original assumption.

We assume the following asymptotic behaviour for the  $\epsilon_k$ 's and the  $\omega_q$ 's:

$$\omega_q(\ell) = \omega_q(\infty) + \frac{b_q}{2\sqrt{\ell}} \quad (4.16)$$

and

$$\epsilon_k(\ell) = \epsilon_k(\infty) + \frac{b_k}{2\sqrt{\ell}}. \quad (4.17)$$

Here the  $b_q$  and  $b_k$  are real functions of  $q$  resp  $k$ , but do not depend on  $\ell$ . The factor  $\frac{1}{2}$  is chosen for convenience only. This asymptotic behaviour was first found for the spin-boson problem by Kehrein, Mielke and Neu [8] and then used by Lenz and Wegner for the flow of the phonons. In our case the electronic flow of the energy is taken into account as well leading to more complicated equations.

We use  $d_{k,q} := b_{k+q} - b_k + b_q$ ,

$$\text{i.e. } \alpha_{k,q}(\ell) = \alpha_{k,q}(\infty) + \frac{b(k+q)}{2\sqrt{\ell}} - \frac{b(k)}{2\sqrt{\ell}} + \frac{b(q)}{2\sqrt{\ell}} = \alpha_{k,q}(\infty) + \frac{d_{k,q}}{2\sqrt{\ell}}. \quad (4.18)$$

We will use  $\alpha_{k,q}(\ell) = \alpha_k(q, \ell) = \alpha_q(k, \ell)$ , as well as  $d_{k,q}(\ell) = d_k(q, \ell) = d_q(k, \ell)$  to demonstrate which variable is part of the integral. We also put  $\alpha_{k,q}(\infty) =: \alpha_{k,q}$

To calculate 4.15 we choose appropriate coordinates, i.e. the  $z$ -direction in  $q$  space is chosen parallel to  $k$ .

$$\begin{aligned} & \int_B d^3 q \alpha_{k,q}(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \\ &= \int_B d^3 q |M_q|^2 \left( \alpha_k(q, \infty) + \frac{d_k(q)}{2\sqrt{\ell}} \right) e^{-2(\ell \alpha_k^2(q, \infty) + 2\alpha_k(q, \infty) d_k(q) \sqrt{\ell} + \frac{d_k^2(q)}{4} \ln \ell)}. \end{aligned} \quad (4.19)$$

Here we did not take into account the last term at the lower boundary of the  $\ell$ -integral, i.e. we put:  $\int_0^\ell \frac{d^2}{4} \frac{1}{\ell'} d\ell' = \frac{d^2}{4} \ln \ell$  and dropped the term: " $\frac{d^2}{\ln 0}$ ". This problem can be solved by either restricting the  $\ell$ -integral to the asymptotic regime  $\int_{\ell_0}^\ell$  or by using an asymptotic behaviour of the kind:  $\frac{d}{\sqrt{\ell + \ell_0}}$  which will be done in chapter 5.4. Expression (4.19) gives:

$$\begin{aligned} & \int_B d^3 q |M_q|^2 \left( \alpha_k(q, \infty) + \frac{d_k(q)}{2\sqrt{\ell}} \right) \ell^{-\frac{1}{2} d_k^2(q)} e^{2d_k^2(q)} e^{-2\ell(\alpha_k(q, \infty) + \frac{d_k(q)}{\sqrt{\ell}})^2} \\ &= 2\pi \int_B q dq dq_z |M_q|^2 \left( \alpha_k(q, q_z, \infty) + \frac{d_k(q, q_z)}{2\sqrt{\ell}} \right) \ell^{-\frac{1}{2} d_k^2(q, q_z)} e^{2d_k^2(q, q_z)} e^{-2\ell(\alpha_k(q, q_z, \infty) + \frac{d_k(q, q_z)}{\sqrt{\ell}})^2} \end{aligned} \quad (4.20)$$

We denote  $\alpha_k(q, q_z, \infty) + \frac{d_k(q, q_z)}{\sqrt{\ell}}$  as  $\alpha_k(q, q_z, \infty)$  again and obtain

$$\begin{aligned}
 & 2\pi \int_B q dq dq_z |M_q|^2 \left( \alpha_k(q, q_z, \infty) - \frac{d_k(q, q_z)}{2\sqrt{\ell}} \right) \ell^{-\frac{1}{2}d_k^2(q, q_z)} e^{2d_k^2(q, q_z)} e^{-2\ell(\alpha_k(q, q_z, \infty))^2} \\
 & \Rightarrow -\frac{1}{\ell} \pi \sqrt{\frac{\pi}{2}} \int_B q^2 dq dq_z \tilde{c}^2 d_k(q, q_z) \ell^{-\frac{1}{2}d_k^2(q, q_z)} e^{2d_k^2(q, q_z)} \delta(\alpha_k(q, q_z, \infty)) \quad \text{for } \ell \rightarrow \infty.
 \end{aligned} \tag{4.21}$$

We used  $|M_q| = \tilde{c}\sqrt{q}$  and  $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$ . The above is equivalent to:

$$-\pi \sqrt{\frac{\pi}{2}} \frac{1}{\ell} \tilde{c}^2 \int_{\gamma(t)} q^2(t) d_k(t) \ell^{-\frac{1}{2}d_k^2(t)} e^{2d_k^2(t)} \frac{1}{|\vec{\nabla} \alpha_k(t, \infty)|} dt \tag{4.22}$$

where  $\gamma(t)$  is the curve in the  $q, q_z$ -plane given by  $\alpha_k(q, q_z, \infty) = 0$ .

We now use this result for (4.15) to write down the derivatives of  $\epsilon_k$  and  $\omega_q$  where we calculate the right hand and left hand side of (4.13) and (4.12) separately<sup>1</sup>.

$$\begin{aligned}
 & \frac{d\epsilon_k}{d\ell} = -\frac{b(k)}{4} \frac{1}{\ell^{\frac{3}{2}}} = \quad \quad \quad k > k_f \\
 & = \sqrt{2}\Gamma \frac{1}{\ell} \pi^{\frac{3}{2}} \int_B q dq dq_z \tilde{c}^2 q d_k(q, q_z) \ell^{-\frac{1}{2}d_k^2(q, q_z)} e^{2d_k^2(q, q_z)} \delta(\alpha_k(q, q_z, \infty)) (1 - n_{k+q}) \\
 & = \sqrt{2}\Gamma \pi^{\frac{3}{2}} \frac{1}{\ell} \tilde{c}^2 \int_{\gamma(t)} dt \frac{1}{|\vec{\nabla} \alpha(t)|} (d_k(t)) q^2(t) \ell^{-\frac{1}{2}d_k^2(t)} e^{2d_k^2(t)} (1 - n_{k+q})
 \end{aligned} \tag{4.23}$$

$$\begin{aligned}
 & \frac{d\omega_q}{d\ell} = -\frac{b(q)}{4} \frac{1}{\ell^{\frac{3}{2}}} = \\
 & = -\sqrt{2}\Gamma \frac{1}{\ell} \pi^{\frac{3}{2}} \tilde{c}^2 \int_B k dk dk_z q d_q(k, k_z) \ell^{-\frac{1}{2}d_q^2(k, k_z)} e^{2d_q^2(k, k_z)} \delta(\alpha_q(k, k_z, \infty)) (n_{k+q} - n_k) \\
 & = -\sqrt{2}\Gamma \pi^{\frac{3}{2}} \tilde{c}^2 q \frac{1}{\ell} \int_{\gamma(t)} dt \frac{1}{|\vec{\nabla} \alpha(t)|} (d_q(t)) k(t) \ell^{-\frac{1}{2}d_q^2(t)} e^{2d_q^2(t)} (n_{k+q} - n_k)
 \end{aligned} \tag{4.24}$$

These equations have to be fulfilled in order for our assumption to be self-consistent. The first self consistency test requires the algebraic decay in  $\ell$  to be the same for the right hand and left hand side of these equations. This holds, for example, as long as  $d(k, q) = 1 \quad \forall k, q : \quad \alpha_{k,q}(\infty) = 0$ . Then we have:

$$b(q) \frac{1}{\ell^{\frac{3}{2}}} = 4\sqrt{2}\pi^{\frac{3}{2}} e^2 \Gamma \tilde{c}^2 q \frac{1}{\ell^{\frac{3}{2}}} \int_{\gamma(t)} dt \frac{1}{|\vec{\nabla} \alpha(t)|} k(t) (n_{k+q} - n_k)$$

---

<sup>1</sup>For  $k < k_f$  we have an equivalent equation which is found by simply replacing  $\alpha_{k,q}$  by  $\alpha_{k+q,-q}$



Equations (4.23) and (4.24) take the form:

$$-b(k)\ell^{-\frac{3}{2}} = \tilde{C}(k)\ell^{-\frac{3}{2}} \quad (4.25)$$

$$-b(q)\ell^{-\frac{3}{2}} = -\tilde{C}(q)\ell^{-\frac{3}{2}} \quad (4.26)$$

This shows the condition for  $b(k)$  and  $b(q)$  in order for our assumption on the asymptotic behaviour to be self-consistent. To investigate this further we will use (4.23) and (4.24) to calculate  $\tilde{C}(k)$  and  $\tilde{C}(q)$  and the  $b(k)$  and  $b(q)$ . The larger part of this thesis will then deal with the problem of really meeting this second requirement for self consistency. Before dealing with this main point we make a remark on the algebraic decay.

### 4.3. Showing the inconsistency of other algebraic behaviours

We show that any algebraic decay other than  $\frac{1}{\sqrt{\ell}}$  will fail to meet the first requirement for self consistency.

We assume  $\alpha_k(q, \ell)$  to be of the form:  $\alpha_k(q, \infty) + \frac{d_k(q)}{\ell^\gamma}$ . Here  $\frac{d_k(q)}{\ell^\gamma}$  is the leading term in the asymptotic behaviour as  $(\ell \rightarrow \infty)$ . As soon as  $\gamma$  is given the integrals governing  $\frac{d\epsilon}{d\ell}$  and  $\frac{d\omega}{d\ell}$  yield the same asymptotic behaviour in  $\ell$ , this is why we consider only the integral governing  $\frac{d\epsilon}{d\ell}$ .

We use the same steps as in the case of  $\gamma = \frac{1}{2}$  to calculate the right hand side of (4.13). For the four cases  $\gamma > 1$ ,  $\gamma = 1$ ,  $1 > \gamma > \frac{1}{2}$ ,  $\frac{1}{2} > \gamma > 0$  we compare the  $\ell$ -dependency (as  $\ell \rightarrow \infty$ ) of the left and right hand side of (4.13)

a)  $\gamma > 1$ :

$$\frac{1}{\ell^{\gamma+1}} \text{ versus } \frac{1}{\ell^{\gamma+\frac{1}{2}}} \quad (4.27)$$

b)  $\gamma = 1$ :

$$\frac{1}{\ell^2} \text{ versus } \frac{1}{\ell^{\frac{3}{2}}} \quad (4.28)$$

c)  $1 > \gamma > \frac{1}{2}$

$$\frac{1}{\ell^{\gamma+1}} \text{ versus } \frac{1}{\ell^{\gamma+2}} \quad (4.29)$$

d)  $\frac{1}{2} > \gamma > 0$ :

$$\frac{1}{\ell^{\gamma+1}} \text{ versus } \frac{1}{\ell^{\gamma+\frac{1}{2}}} e^{-const \cdot \ell^{1-2\gamma}} \quad (4.30)$$

We can conclude: The only possible algebraic asymptotic behaviour is given by:

$$\alpha_{k,q}(\ell) = \alpha_{k,q}(\infty) + \frac{d_{k,q}}{2\sqrt{\ell}} \quad (4.31)$$

or:

$$\epsilon_k(\ell) = \epsilon_k(\infty) + \frac{b_k}{2\sqrt{\ell}} \quad (4.32)$$

$$\omega_q(\ell) = \omega_q(\infty) + \frac{b_q}{2\sqrt{\ell}} \quad (4.33)$$

#### 4.4. Decay of the Interaction Constants

In this section we will prove that all parts of the electron-phonon interaction do decay as  $\ell \rightarrow \infty$ . This shows that our choice of  $\eta(\ell)$  does yield a block-diagonal form of our Hamiltonian under the  $\ell$  induced transformation

##### 4.4.1. Exponential Decay away from Resonances

Let  $q$  and  $k$  be values, such that

$|\alpha_{k,q}(\infty)| = |\epsilon_{k,q}(\infty) - \epsilon_k(\infty) + \omega_q(\infty)| =: \tilde{a} \neq 0$ , where  $\tilde{a}$  is some constant. Then there is a  $\ell^*$ , such that for all  $\ell > \ell^*$  we have

$|\alpha(\ell)| = |\alpha(\infty) + \frac{1}{2\sqrt{\ell}}| > \frac{\tilde{a}}{2}$ . Equations (4.1) and (4.31) show that for a given  $\ell > \ell^*$

$$|M_{k,q}(\ell)| < |M_{k,q}(0)| \cdot e^{-\frac{\tilde{a}}{2}(\ell - \ell^*)} \quad (4.34)$$

##### 4.4.2. Algebraic Decay at resonances

For values of  $q$  and  $k$  which belong to resonances, i.e.  $\alpha_{k,q}(\infty) = 0$  we have some  $\ell^*$  such that for all  $\ell > \ell^*$ :  $\alpha_{k,q}(\ell) = \frac{1}{2\sqrt{\ell}}$ . We then integrate (4.1) and find

$$|M_{k,q}(\ell)| < |M_{k,q}(0)| \cdot e^{-\frac{1}{4} \ln \ell} = |M_{k,q}(0)| \cdot \ell^{-\frac{1}{4}} \quad (4.35)$$

This shows the decay of all interaction constants under the  $\ell$  induced transformation.

## 5. Further Investigations on the Asymptotic Behaviour

We have seen in the last chapter that the assumption of a  $\frac{const}{\sqrt{\ell}}$  behaviour is the only possible algebraic flow for a self consistent solution. In this chapter we search for the coefficients  $b(q)$  and  $b(k)$ , to find a fully self-consistent solution of (4.23) and (4.24). In the first section, we will make some remarks on the behaviour of the  $\epsilon(k)$  and  $\omega(q)$  under the  $\ell$  induced transformation. In the second section we investigate the derivatives of the  $\omega_q(\ell)$  and  $\epsilon_k(\ell)$  for  $b(q)$  and  $b(k)$  being independent of  $q$  and  $k$ , respectively. This corresponds to the unperturbed phononic flow. We then evaluate the integrals determining the  $b(q)$  and  $b(k)$  under the assumption  $d_{k,q} = b(k+q) - b(k) + b(q) = 1$  in section 5.3. The results give a hint on how to continue our considerations. We are lead to use a more specific ansatz as used by Wegner and Ragwitz [7] who correctly described the asymptotic behaviour of the phononic flow under the assumption of constant electronic energies.

In section 5.4 we will use  $\omega_q(\ell) = \omega_q(\infty) + \frac{b(q)}{2\sqrt{\ell+\ell_0}}$  and a similar form for the electronic flow to find the form of the  $b(q)$  and  $b(k)$  for a self consistent solution. In the last section of this chapter we present a self-consistent solution and discuss its physical implications.

For  $T = 0$  the important effects are going to be those involving small  $q$  and values of  $k$  near to  $k_f$ . For this reason we will expand, if necessary, in terms of  $q$  and  $k - k_f$ .

### 5.1. General Considerations

For the deduction of the general asymptotic behaviour in the last chapter, we used the assumption (see Appendix A), that during the  $\ell$ -dependent transformation a crossing of the electronic energy levels does not occur. This means for all  $\ell$ :

$$k > k' \Leftrightarrow \epsilon_k(\ell) > \epsilon_{k'}(\ell)$$

As the  $\omega_q$  are phononic, i.e. bosonic energies we further assume:

$$\omega_q(\ell) \geq 0 \quad \forall \ell, q$$

To obtain  $\alpha_{k,q}(\ell) = \epsilon_{k+q}(\ell) - \epsilon_k(\ell) + \omega_q(\ell) = 0$  we then need:

$$q = 0 \quad \text{or} \quad |k+q| < k$$

Take a look at the equations (4.12), (4.13) and (4.14). We want to find those parts of these integrals, which are important for the algebraic decay in the asymptotic regime. That is, those regions in which  $\alpha_{k,q}(\infty) = 0$ , because of the exponential suppression for other  $\alpha$ .

We start with the integral for the evaluation of  $\frac{d\omega}{d\ell}$ . The regions over which this integral is taken, are given by:

$$\begin{aligned} n_{k+q} = 1 \quad \text{and} \quad n_k = 0 \\ \text{or} \\ n_{k+q} = 0 \quad \text{and} \quad n_k = 1. \end{aligned}$$

In the second case, we would have:  $\alpha_{k,q}(\ell) = \epsilon_{k+q}(\ell) - \epsilon_k(\ell) + \omega_q(\ell) > \omega_q(\ell) > 0$ , which leads to a term exponentially decaying, compared to the leading asymptotic behaviour. The integral in (4.13) differs from zero only if  $n_{k+q} = 0$ , that is, we have  $|k+q| > k_f$ . Let  $k < k_f$ , this means:  $\epsilon_{k+q} - \epsilon_k + \omega_q > \epsilon_{k_f} - \epsilon_k + \omega_q > \text{const} > 0$ . This integral is exponentially decaying with  $\ell$  for all  $k$  smaller than  $k_f$ .

Whereas in (4.14) we have  $|k+q| < k_f$  and, as the significant region of integration is given by:  $\alpha_{k+q,-q} = \epsilon_k - \epsilon_{k+q} + \omega_q = 0$ , we find  $\alpha_{k+q,-q} > \epsilon_k - \epsilon_{k_f} + \omega_q > \text{const} > 0$  for any  $k$  above the fermi surface. And this integral is exponentially decaying for all  $k$  larger than  $k_f$ .

The parts of the integrals (4.12)-(4.14), which contribute to the algebraic decay, are given by:

$$\frac{d\omega_q}{d\ell} : \quad |k+q| < k_f < k \quad (5.1)$$

$$\frac{d\epsilon_k}{d\ell} : \quad k > |k+q| > k_f; \quad \frac{d\epsilon_k}{d\ell} : \quad k < |k+q| < k_f \quad (5.2)$$

## 5.2. Example 1: Unperturbed Phononic Flow

To get a feeling for equations (4.12)-(4.14) we discuss a very simple assumption<sup>1</sup>. Lets take  $d_{k,q}$  to be a constant, i.e.  $d = b(k+q) - b(k) + b(q) = 1$ . Then we have (see 4.23 and 4.24)<sup>2</sup>:

$$\begin{aligned} \frac{d\omega_q}{d\ell} &= -\frac{b(q)}{4} \frac{1}{\ell^{\frac{3}{2}}} \\ &= -\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2q\frac{1}{\ell^{\frac{3}{2}}} \int_B kdkdk_z \delta(\alpha_q(k, k_z, \infty))(n_{k+q} - n_k) \end{aligned}$$

---

<sup>1</sup>N.B. In general the  $b(q)$  and  $b(k)$  are two distinct functions

<sup>2</sup>N.B. None of the remaining integrals is  $\ell$  dependent

$$= -\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2q\frac{1}{\ell^{\frac{3}{2}}}\int_{\gamma(t)} dt k(t)\frac{1}{|\vec{\nabla}\alpha(t)|}(n_{k+q}-n_k) \quad (5.3)$$

$$\begin{aligned} \frac{d\epsilon_k}{d\ell} &= -\frac{b(k)}{4}\frac{1}{\ell^{\frac{3}{2}}} & k > k_f \\ &= \sqrt{2}\Gamma e^2\pi^{\frac{3}{2}}\tilde{c}\frac{1}{\ell^{\frac{3}{2}}}\int_B q^2 dq dq_z \delta(\alpha_k(q, q_z, \infty))(1-n_{k+q}) \\ &= \sqrt{2}\Gamma e^2\pi^{\frac{3}{2}}\tilde{c}\frac{1}{\ell^{\frac{3}{2}}}\int_{\gamma(t)} dt q^2(t)\frac{1}{|\vec{\nabla}\alpha(t)|}(1-n_{k+q}) \end{aligned} \quad (5.4)$$

We will discuss these equation for very simple forms of the  $b(k)$ s and  $b(q)$ s. A natural first try is to choose the  $b(q)$  and  $b(k)$  as constants. As one can see, the derivatives of the electronic energies change sign at the fermi surface. (4.13)+(4.14). That is why we assume  $b(k)$  to change sign at the fermi surface. For didactical reasons we will also investigate the case of constant  $b(k)$ :

I)  $b(q) = A$ ,  $b(k) = B$   $k > k_f$  and  $b(k) = -B$   $k < k_f$ , will be our first try.

II) In addition we will take a look at:  $b(q) = A$ ,  $b(k) = B$

This would mean, the inclusion of the electronic flow does not alter the phononic flow. As for the phononic flow both these choices yield the same asymptotic behaviour, as obtained by Wegner and Lenz [5], who neglected the effects of the electronic-flow. This can be described simply by setting  $B = 0$ .

We check, whether these assumptions can be self-consistent in our considerations, where the flow of the electronic energies is included. For the first assumption we explicitly have:

$$\begin{aligned} \epsilon_k(\ell) &= \epsilon_k(\infty) + \frac{B}{2\sqrt{\ell}}, & k > k_f \\ \epsilon_k(\ell) &= \epsilon_k(\infty) - \frac{B}{2\sqrt{\ell}}, & k < k_f \\ \omega_q(\ell) &= \omega_q(\infty) + \frac{A}{2\sqrt{\ell}}, & k > k_f \end{aligned} \quad (5.5)$$

Consider further the integral governing  $\frac{d\omega_q}{d\ell}$ . The integral splits into two parts. As we have argued in (5.1) only one part, given by:  $|k+q| < k_f < k$  is important for our investigation of the asymptotic behaviour. This lead to:  $\alpha_{k,q}(\ell) = \alpha_{k,q}(\infty) + \frac{-2B+A}{2\sqrt{\ell}}$ , thus:

$$d = -2B + A.$$

Within the region of integration in (5.4), it is easily seen, that  $|k+q|, k > k_f$  and this means  $\alpha_{k,q}(\ell) = \alpha_{k,q}(\infty) + \frac{B-B+A}{2\sqrt{\ell}} \Rightarrow d = A$ . Combining both of these conditions gives

$B = 0$ . This means  $\frac{d\epsilon}{d\ell} = 0$ , which is not possible.

For the second case, i.e. II) we have  $A = 1$  for all our integrals. But, as argued above, the resulting derivatives of the electronic energies change sign at the fermi surface.

Further, take a look at the equation (5.4), with  $|k|$  only slightly bigger, than  $k_f$ . For  $\alpha$  to be zero  $|k + q|$  has to be smaller than  $|k|$  and at the same time bigger than  $k_f$  for (5.4) to be non zero. Thus the set  $S$  (zeros of  $\alpha_{k,q}$ ), i.e. the region of integration over  $dt$  in (5.4), will decline like  $(k - k_f)^2$  as  $k \rightarrow k_f$ . This contradicts the assumption of  $B$  beeing a constant.

Easy solutions for our set of equations cannot be found, even not in the asymptotic regime. To get an idea on how to continue our considerations, we will use,  $d=1$  to calculate  $b(q)$  and  $b(k)$ .

### 5.3. First Calculation of the $b_k$ and $b_q$

We assume an asymptotic behaviour as given in 4:

$$\omega_q(\ell) = \omega_q(\infty) + \frac{b_q}{2\sqrt{\ell}} \quad \epsilon_k(\ell) = \epsilon_k(\infty) + \frac{b_k}{2\sqrt{\ell}} \quad (5.6)$$

Instead of assuming  $b_q$  and  $b_k$  to be constant we use equations (5.3) and (5.4), in a form, where the azimuthal symmetry hasn't yet been integrated over, to calculate  $b_q$  and  $b_k$ . As long as:  $b(k + q) - b(k) + b(q) = d_{k,q} = 1$  for all  $k, q : \alpha_{k,q} = 0$  we have:

$$-\frac{b(q)}{4} = -\frac{1}{\sqrt{2}}\Gamma\sqrt{\pi}e^2\tilde{c}^2q \int_B \delta(\alpha_q(k))(n_{k+q} - n_k)d^3k \quad (5.7)$$

and

$$-\frac{b(k)}{4} = \frac{1}{\sqrt{2}}\Gamma\sqrt{\pi}e^2\tilde{c}^2 \int_B q\delta(\alpha_k(q))(1 - n_{k+q})d^3q \quad k > k_f \quad (5.8)$$

$$-\frac{b(k)}{4} = -\frac{1}{\sqrt{2}}\Gamma\sqrt{\pi}e^2\tilde{c}^2 \int_B q\delta(\alpha_{k+q,-q}(q))n_{k+q}d^3q \quad k < k_f \quad (5.9)$$

To solve these expressions we assume, that  $\alpha_{k,q}$  does not change significantly under the flow of  $\ell$ , this is:  $\delta(\alpha_{k,q}(\infty)) = \delta(\alpha_{k,q}(0))$ .

#### 5.3.1. Evaluation of $b(q)$

As we have shown in the previous section, our region of integration for (5.7) is given by:

$$k > k_f > |k + q|, \quad (5.10)$$

We choose the  $z$ -axis of  $\vec{k}$  antiparallel to  $\vec{q}$ , and with  $q = |\vec{q}|$  we have:

$$\alpha_q(k) = \frac{q^2}{2m} - \frac{k_z q}{m} + cq = 0 \quad (5.11)$$

Setting  $r^2 = k_x^2 + k_y^2$ , we evaluate (5.7):

$$\begin{aligned} b(q) &= 2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2q \int_B d^3k (n_{k+q} - n_k) \delta(\alpha_q(k)) = \\ &= 4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2q \int_B r dr dk_z (n_{k+q} - n_k) \delta\left(\frac{q^2}{2m} - \frac{k_z q}{m} + cq\right) \end{aligned}$$

Due to (5.10)

$$(k_z - q)^2 + r^2 < k_f^2 < k_z^2 + r^2 \quad \text{which leads to} \quad 0 < k_z < k_f + q$$

We split the integral into two parts

$$\begin{aligned} &4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2q \int_0^{k_f} \int_{\sqrt{k_f^2 - k_z^2}}^{\sqrt{k_f^2 - (k_z - q)^2}} r dr dk_z \delta\left(\frac{q^2}{2m} - \frac{k_z q}{m} + cq\right) \\ &4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2q \int_{k_f}^{k_f + q} \int_0^{\sqrt{k_f^2 - (k_z - q)^2}} r dr dk_z \delta\left(\frac{q^2}{2m} - \frac{k_z q}{m} + cq\right) \end{aligned}$$

As  $q$  is small and  $c$  is small compared to  $\frac{k_f}{m}$ , the argument of the  $\delta$ -function in the second integral never vanishes. We substitute variables  $y = \frac{k_z q}{m}$  and continue the calculation for the first integral:

$$4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2q \int_0^{k_f} \frac{q}{m} \int_{\sqrt{k_f^2 - \frac{m^2}{q^2}y^2}}^{\sqrt{k_f^2 - (\frac{m}{q}y - q)^2}} r dr dy \frac{m}{q} \delta\left(\frac{q^2}{2m} - y + cq\right) = \quad (5.12)$$

$$4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2m \int_0^{k_f} \frac{q}{m} F(y) dy \delta\left(\frac{q^2}{2m} - y + cq\right)$$

Straight forward integration over  $r$  and then over  $y$  yields:

$$b(q) = 4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2m^2cq \quad (5.13)$$

$$\text{i.e.} \quad b(q) = \text{const} \cdot q \quad (5.14)$$

where

$$\text{const} = 4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2m^2 \quad (5.15)$$

### 5.3.2. Evaluation of $\mathbf{b}(\mathbf{k})$

We now want to investigate the behaviour of the electronic energies near the fermi surface. (Explicitely we only consider values of  $k > k_f$ ).

Again choosing suitable integration variables for our integral, we assume the z-axis of our q-integral to be parallel to  $\vec{k}$ . We then have:

$$\begin{aligned}\alpha_k(q) &= \frac{q^2}{2m} + \frac{q_z k}{m} + c|q| = 0 \quad \text{which requires } q_z < 0 \\ &\rightarrow |q| = -mc + \sqrt{m^2 c^2 - 2q_z k},\end{aligned}\tag{5.16}$$

The region of integration is limited by:

$$\begin{aligned}(1 - n_{k+q}) &= 1 \\ \text{which gives } k^2 + 2kq_z + q^2 &> k_f^2 \quad \text{or} \quad q^2 > k_f^2 - k^2 - 2kq_z\end{aligned}\tag{5.17}$$

This condition and  $\alpha_{k,q} = 0$  can only be fulfilled as long as  $q_z$  is smaller than the value calculated below.

$$\begin{aligned}k_f^2 - k^2 - 2kq_z &= q^2 = m^2 c^2 + m^2 c^2 - 2kq_z - 2mc\sqrt{m^2 c^2 - 2kq_z} \\ &\text{which leads to} \\ q_z &= \frac{1}{2k}(k_f^2 - k^2) - \frac{1}{8m^2 c^2 k}(k_f^2 - k^2)^2 := -a\end{aligned}\tag{5.18}$$

As we are interested in values of  $k$  near the fermi surface, the last line can be approximated to yield:

$$a = (k - k_f)$$

We only have to take into account those parts of the integral with  $0 > q_z > -a$ . We change coordinates of our integral to  $q_z$  and  $q$ . Then the lower boundary  $l_l$  of the  $q$  part is given by the larger value of  $|q_z|$  and  $\sqrt{\max\{0, k_f^2 - k^2 - 2kq_z\}}$ .



We proceed with the calculation of (5.4):

$$\begin{aligned}
 -\frac{b(k)}{4} &= \frac{1}{\sqrt{2}}\Gamma\sqrt{\pi}e^2\tilde{c}^2 \int_B d^3q q \delta(\alpha_k(q))(1 - n_{k+q}) \Rightarrow \\
 b(k) &= -2\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \int_{l_i}^B dq q^2 \delta(\alpha_k(q, q_z, \infty)) \\
 &= -2\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \int_{l_i}^B dq q^2 \frac{1}{(\frac{q}{m}+c)} \delta(q + mc - \sqrt{m^2c^2 - 2kq_z}) \\
 &= -2\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z (-mc + \sqrt{m^2c^2 - 2kq_z})^2 \frac{m}{(\sqrt{m^2c^2 - 2kq_z})} \\
 &= -2\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \left( \frac{2m^3c^2 - 2mkq_z}{\sqrt{m^2c^2 - 2kq_z}} - 2m^2c \right)
 \end{aligned} \tag{5.19}$$

We are interested in the change of the electronic energies near the fermi surface, then  $|q_z| \leq a$ , which itself is of the order of  $k - k_f$ , is small. Expanding the denominator, we find:

$$\begin{aligned}
 &= -2\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z (2m^3c^2 - 2mkq_z) \frac{1}{mc} \left( 1 + \frac{k}{m^2c^2}q_z + \frac{3}{2}\frac{k^2}{m^4c^4}q_z^2 \right) - 2m^2c \\
 &= -2\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \frac{k^2}{m^2c^3}q_z^2 \\
 &= -\frac{2}{3}\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \frac{k^2}{m^2c^3}a^3
 \end{aligned} \tag{5.20}$$

As

$$a = \frac{1}{2}(k^2 - k_f^2) + \frac{1}{8m^2c^2k}(k_f^2 - k^2)^2 \approx k_f(k - k_f),$$

it is easily seen, that:

$$b(k) = -const(k - k_f)^3 \tag{5.21}$$

These calculations show, that assuming  $d = 1$  and a behaviour like  $\omega, \epsilon \sim \frac{const}{\sqrt{\ell}}$  for all  $\ell$  would lead to a contradiction as e.g.  $d_{k,q} \rightarrow 0$  for  $|q| \rightarrow 0$ . Trying to fix this problem, we will now take into account a different dependence on  $\ell$  for smaller values of  $\ell$ .

## 5.4. A shifted Asymptotic Behaviour: $\frac{1}{2\sqrt{\ell+\ell_0}}$

Until now we have assumed the asymptotic forms (4.32) and (4.33) for all values of  $\ell$ , which gave rise to the singularities discussed in section 4.2. When assuming a shifted

asymptotic behaviour, the difficulty disappears. In the last section we have seen, that a major problem in obtaining a self consistent solution is the problem of finding values of  $b_k$  and  $b_q$ , such that  $d_{k,q}$  equals one.

This problem exists even if only the phononic flow is considered, i.e.  $\epsilon_k(\ell) = \epsilon_k(\infty) = \epsilon_k(0)$ . In this case,  $d_q = b(q) = 1$  is needed. Wegner and Ragwitz[7] solved this problem by including the onset of the asymptotic behaviour. Instead of setting

$$\omega_q(\ell) = \omega_q(\infty) + \frac{1}{2\sqrt{\ell}} \quad (5.22)$$

they used:

$$\omega_q(\ell) = \omega_q(\infty) + \frac{1}{2\sqrt{\ell + \ell_0}} \quad (5.23)$$

where  $\ell_0 = \frac{1}{(4\Gamma\tilde{c}^2\omega_q(\infty)\sqrt{\frac{\pi}{2}}e^2)^2}$ .

As  $\sqrt{\ell_0}$  has a pole at  $q = 0$ , we loose one power of  $q$  in (5.13), which leads to  $b(q)=d=1$ , and thus solves (4.12) self-consistently, as long as the electronic flow is neglected.

The new behaviour of the flow can be interpreted as follows: For small  $\ell \ll \ell_0$ , the one particle energies are nearly constant. For  $\ell \approx \ell_0$  there is an intermediate region and finally for  $\ell \gg \ell_0$  the general asymptotic behaviour is refound.

It makes good sense to assume a very similar asymptotic behaviour for the phononic flow, even if the effects of the electronic flow are included. The change of the electronic dispersion relation is small and hence. this change does not alter the phononic flow dramatically. For this reason, we assume the asymptotic behaviour of the phononic and electronic flow to be of this shifted form.

$$\omega_q(\ell) = \omega_q(\infty) + \frac{b_q}{2\sqrt{\ell + \ell_0(q)}} \quad \epsilon_k(\ell) = \epsilon_k(\infty) + \frac{b_k}{2\sqrt{\ell + \ell_\epsilon(k)}} \quad (5.24)$$

Still assuming  $d_{k,q} = 1 \quad \forall k, q : \alpha_{k,q}(\infty) = 0$ , we now do the same calculations as in chapter 4:

$$\begin{aligned} -\frac{b(q)}{4} \frac{1}{\sqrt{\ell + \ell_0(q)}^3} &= 2\Gamma \int_B d^3k \alpha_q(k, \ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_q^2(k, \ell') d\ell'} (n_{k+q} - n_k) \\ &= 2\Gamma \int_B d^3k (\alpha_q(k, \infty) + \sum_i \frac{b_i}{2\sqrt{\ell + \ell_i}}) |M_q|^2 e^{-2 \int_0^\ell (\alpha_q(k, \infty) + \sum_i \frac{b_i}{2\sqrt{\ell' + \ell_i}})^2 d\ell'} (n_{k+q} - n_k) \end{aligned} \quad (5.25)$$

where we put

$$\ell_1 := \ell_\epsilon(k + q), \ell_2 := \ell_\epsilon(k), \ell_3 := \ell_0(q); \quad b_1 := b(k + q), b_2 := -b(k), b_3 := b(q)$$

We calculate the exponent (using  $\alpha_{q,k} := \alpha_{q,k}(\infty)$ ):

$$\begin{aligned}
 & -2 \int_0^\ell (\alpha_{q,k} + \sum_i \frac{b_i}{2\sqrt{\ell'+\ell_i}})^2 d\ell' \\
 & = -2 (\alpha_q(k)^2 \ell + 2\alpha_q(k) \sum_i b_i \sqrt{\ell + \ell_i} - 2\alpha_q(k) \sum_i b_i \sqrt{\ell_i}) \\
 & - \sum_i \frac{1}{2} b_i^2 \ln(\ell + \ell_i) - \frac{1}{2} \sum_{i \neq j} b_i b_j \ln(\ell + \frac{1}{2}(\ell_i + \ell_j) + \sqrt{\ell^2 + (\ell_i + \ell_j)\ell + \ell_i \ell_j}) \\
 & + \frac{1}{2} \sum_i b_i^2 \ln \ell_i + \frac{1}{2} \sum_{i \neq j} b_i b_j \ln(\frac{1}{2}(\ell_i + \ell_j) + \sqrt{\ell_i \ell_j})
 \end{aligned} \tag{5.26}$$

we set  $\ell + \ell_i \approx \ell$  and find<sup>3</sup>:

$$\begin{aligned}
 & = -2\ell(\alpha_{q,k} + \sum_i \frac{b_i}{\sqrt{\ell}})^2 + 2(\sum_i b_i)^2 \\
 & + 4\alpha_{q,k} \sum_i b_i \sqrt{\ell_i} \\
 & - \sum_i \frac{1}{2} b_i^2 \ln(\ell) - \frac{1}{2} \sum_{i \neq j} b_i b_j \ln(\ell) \\
 & + \frac{1}{2} \sum_i b_i^2 \ln \ell_i + \frac{1}{2} \sum_{i \neq j} b_i b_j \ln(\frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2}\sqrt{\ell_i \ell_j})
 \end{aligned} \tag{5.27}$$

We set  $\ell + \ell_0 \approx \ell$  for the left hand side of (5.3) as well and find for the phononic flow:

$$\begin{aligned}
 & -\frac{b(q)}{4} \frac{1}{\sqrt{\ell}^3} = 2\Gamma \int_B (\alpha_q(k) + \sum_i \frac{b_i}{2\sqrt{\ell}}) |M_q|^2 e^{-2\ell(\alpha_q(k) + \sum_i \frac{b_i}{\sqrt{\ell}})^2} e^{2(\sum_i b_i)^2} \\
 & \times e^{4\alpha_q(k) \sum_i b_i \sqrt{\ell_i}} \ell^{-\frac{1}{2}(\sum_i b_i)^2} \prod_i \ell_i^{\frac{b_i^2}{2}} \prod_{i \neq j} (\frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2}\sqrt{\ell_i \ell_j})^{\frac{1}{2}b_i b_j} (n_{k+q} - n_k) d^3 k
 \end{aligned} \tag{5.28}$$

We perform the integration over the k-values using the same transformation as in the previous chapter:

$$\begin{aligned}
 b(q) & = 2\sqrt{2}\Gamma \sqrt{\pi} e^2 \tilde{c}^2 q \int_B \delta(\alpha_{q,k})(n_{k+q} - n_k) \\
 & \times \prod_{i \neq j} (\frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2}\sqrt{\ell_i \ell_j})^{\frac{1}{2}b_i b_j} \ell_1^{\frac{1}{2}b_1^2} \ell_2^{\frac{1}{2}b_2^2} \ell_3^{\frac{1}{2}b_3^2} d^3 k
 \end{aligned} \tag{5.29}$$

---

<sup>3</sup>This approximation is only true for the asymptotic region. As long as the  $\ell_0$  and  $\ell_\epsilon$  are no more singular than a pole, the integral over the region, where we are not in the asymptotic regime, does not contribute to the leading order.

where we used:  $\sum_i b_i = d_{k,q} = 1$ .

It is easily seen, that for  $k > k_f$  the derivatives for the electronic energies are given by:

$$\begin{aligned}
 -\frac{b(k)}{4} \frac{1}{\sqrt{\ell}^3} &= -2\Gamma \int_B d^3 q \alpha_k(q, \ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_k^2(q, \ell') d\ell'} (1 - n_{k+q}) \\
 &\Rightarrow \\
 b(k) &= -2\sqrt{2}\Gamma \sqrt{\pi} e^2 \tilde{c}^2 \sqrt{\ell} \int_B |q| d_k(q) \ell^{-\frac{1}{2} d_k^2(q)} \delta(\alpha_k(q)) (1 - n_{k+q}) \\
 &\quad \times \prod_{i \neq j} \left( \frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2} \sqrt{\ell_i \ell_j} \right)^{\frac{1}{2} b_i b_j} \ell_1^{\frac{1}{2} b_1^2} \ell_2^{\frac{1}{2} b_2^2} \ell_3^{\frac{1}{2} b_3^2} d^3 q \Rightarrow \\
 b(k) &= -2\sqrt{2}\Gamma \sqrt{\pi} e^2 \tilde{c}^2 \int_B |q| \delta(\alpha_k(q)) (1 - n_{k+q}) \\
 &\quad \times \prod_{i \neq j} \left( \frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2} \sqrt{\ell_i \ell_j} \right)^{\frac{1}{2} b_i b_j} \ell_1^{\frac{1}{2} b_1^2} \ell_2^{\frac{1}{2} b_2^2} \ell_3^{\frac{1}{2} b_3^2} d^3 q
 \end{aligned} \tag{5.30}$$

For  $k < k_f$  we find:

$$\begin{aligned}
 -\frac{b(k)}{4} \frac{1}{\sqrt{\ell}^3} &= 2\Gamma \int_B d^3 q \alpha_{k+q, -q}(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_{k+q, -q}^2(\ell') d\ell'} n_{k+q} \\
 &\Rightarrow \\
 b(k) &= 2\sqrt{2}\Gamma \sqrt{\pi} e^2 \tilde{c}^2 \int_B |q| \delta(\alpha_{k+q, -q}(q)) n_{k+q} \\
 &\quad \times \prod_{i \neq j} \left( \frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2} \sqrt{\ell_i \ell_j} \right)^{\frac{1}{2} b_i b_j} \ell_1^{\frac{1}{2} b_1^2} \ell_2^{\frac{1}{2} b_2^2} \ell_3^{\frac{1}{2} b_3^2} d^3 q
 \end{aligned} \tag{5.31}$$

where for this last case

$$\ell_1 := \ell_\epsilon(k), \ell_2 := \ell_\epsilon(k+q), \ell_3 := \ell_0(q); \quad b_1 := b(k), b_2 := -b(k+q), b_3 := b(q)$$

Using the experience we have gathered in the proceeding sections (e.g. equations ((5.14) and (5.21)), we make the following ansatz:

$$\begin{aligned}
 b(q) &= 1 + A_1 |q| \quad b(k) = B \cdot (k - k_f) \cdot |k - k_f| \\
 &\text{and} \\
 \sqrt{\ell_0(q)} &= \frac{D_{-1}}{|q|} + D_0 \quad \sqrt{\ell_\epsilon(k)} = E_1 f(k - k_f)
 \end{aligned} \tag{5.32}$$

We are interested in the behaviour of our system for small  $q$  and near the fermi surface, i.e.  $k - k_f$  small. In this regime  $||k + q| - k_f|$  is small as well. In this sense we neglect terms of higher order in  $q$  and  $k - k_f$ .

In (5.32)  $f$  is an arbitrary function of  $k - k_f$ . We only assume, that the behaviour of  $\frac{1}{f}$  for  $k \rightarrow k_f$  can be no more singular than a pole.

### 5.4.1. Calculation of $b(q)$

In this realm we find for (5.29):

$$\begin{aligned}
 b(q) &= 2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2q \int_B \delta(\alpha_q(k))(n_{k+q} - n_k) \\
 &\times \sqrt{\ell_1}^{b_1^2} \sqrt{\ell_2}^{b_2^2} \sqrt{\ell_3}^{b_3^2} \prod_{i < j} \left( \frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2}\sqrt{\ell_i \ell_j} \right)^{b_i b_j} d^3 k \\
 &= 2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2 \mid q \mid \int_B d^3 k \delta(\alpha_q(k)) (n_{k+q} - n_k) \\
 &\times \left( \frac{D-1}{|q|} + D_0 \right)^{1+2A_1|q|} \\
 &\times (E_1 f(\mid k + q \mid - k_f))^{B^2(|k+q|-k_f)^4} \cdot (E_1 f(k - k_f))^{B^2(k-k_f)^4} \\
 &\times \left( \frac{1}{4}(E_1^2 f^2(\mid k + q \mid - k_f) + \left(\frac{D-1}{|q|} + D_0\right)^2) \right. \\
 &\quad \left. + \frac{1}{2}(E_1 f(\mid k + q \mid - k_f))\left(\frac{D-1}{|q|} + D_0\right) \right)^{(1+A_1|q|)(B(|k+q|-k_f)|k+q|-k_f|)} \quad (5.33) \\
 &\times \left( \frac{1}{4}(E_1^2 f^2(k - k_f) + \left(\frac{D-1}{|q|} + D_0\right)^2) \right. \\
 &\quad \left. + \frac{1}{2}(E_1 f(k - k_f))\left(\frac{D-1}{|q|} + D_0\right) \right)^{-(1+A_1|q|)(B(k-k_f)|k-k_f|)} \\
 &\times \left( \frac{1}{4}(E_1^2 f^2(\mid k + q \mid - k_f) + E_1^2 f^2(k - k_f)) \right. \\
 &\quad \left. + \frac{1}{2}(E_1 f(\mid k + q \mid - k_f))(E_1 f(k - k_f)) \right)^{-(B(k-k_f)|k-k_f|)(B(|k+q|-k_f)|k+q|-k_f|)} \\
 &= 2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2q \left( \frac{D-1}{q} + D_0 \right)^{1+2A_1|q|} \\
 &\times \int_B \delta(\alpha_q(k)) (n_{k+q} - n_k) d^3 k (1 + O(q^2, (k - k_f)^2))
 \end{aligned}$$

With  $O(q^2, (k - k_f)^2)$  we denote terms of order  $q^2$ ,  $(k - k_f)^2$ ,  $q(k - k_f)$  or higher as  $q \rightarrow 0$  and  $k \rightarrow k_f$ , eventually multiplied with a logarithmic divergence of the type  $\ln \frac{1}{f}$

for  $k \rightarrow k_f$

These terms of higher order can be found by noting for example:

$$\begin{aligned}
 & h(q, k - k_f)^{(1+A(|q|))(B(|k+q|-k_f)||k+q|-k_f|+B(k-k_f)|k-k_f|)} = \\
 & 1 + (\ln h(q, k - k_f))(B(|k+q|-k_f)||k+q|-k_f|+B(k-k_f)|k-k_f|)) \quad (5.34) \\
 & + h.o.T.
 \end{aligned}$$

$h(q, k - k_f)$  denotes any of the brackets of the last terms in (5.33).

As long as  $h(q, k - k_f)$  is continuous or has poles for  $k \rightarrow k_f$ , it is readily seen, that the second term of (5.34) vanishes like  $o(q)$  and  $o(k - k_f)$ .

We use the same manipulations as in (5.19), to continue from (5.33):

$$\begin{aligned}
 b(q) &= 4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2m \cdot \left(\frac{D_{-1}}{|q|} + D_0\right)^{1+2A_1|q|} \\
 &\times \int \frac{\sqrt{k_f^2 - \frac{q^2}{4} - m^2c^2 + qmc}}{\sqrt{k_f^2 - \frac{q^2}{4} - m^2c^2 - qmc}} (1 + O(q^2, (k - k_f)^2)) r dr \\
 &= 4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2m \left(\frac{D_{-1}}{|q|} + D_0 + A_1 \ln\left(\frac{D_{-1}}{|q|} + D_0\right)q + O(q^2)\right) \\
 &\quad (mcq + O(q^3)) \quad (5.35)
 \end{aligned}$$

Finally our considerations yield:

$$b(q) = 4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2m^2c(D_{-1} + D_0q) + O(q^2) \quad (5.36)$$

We now choose

$$D_{-1} = \frac{1}{4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2m^2c} \quad \text{and} \quad D_0^* = D_0/D_{-1}. \quad (5.37)$$

Then we have:

$$b(q) = 1 + D_0^*q + O(q^2) \quad (5.38)$$

this means:

$$A_1 = D_0^* \quad (5.39)$$

### 5.4.2. Calculation of $b(k)$

We now calculate the  $b(k)$  for  $k > k_f$ . The results for  $k < k_f$  are found analogously.

$$b(k) = -2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2 \int_B |q| \delta(\alpha_k(q))(1 - n_{k+q}) \quad (5.40)$$

$$\times \sqrt{\ell_1}^{b_1^2} \sqrt{\ell_2}^{b_2^2} \sqrt{\ell_3}^{b_3^2} \prod_{i < j} \left( \frac{1}{4}(\ell_i + \ell_j) + \frac{1}{2}\sqrt{\ell_i \ell_j} \right)^{b_i b_j} d^3 q$$

$$= -4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \int dq q^2 \frac{1}{\frac{q}{m}+c} \delta(|q| + mc - \sqrt{m^2 c^2 - 2q_z k})$$

$$\times \left( \frac{D_{-1}}{|q|} + D_0 \right)^{1+A_1|q|} \quad (5.41)$$

$$+ h.o.T.$$

where the higher order terms are again of the form as in (5.34). For the  $q$  integration we have omitted the boundaries (they are the same as given in 5.19), it is only important to note, that the lower boundary is less than zero and the upper boundary is larger than zero. We can write the expression (5.41) as:

$$-4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \int dq q^2 \frac{1}{\frac{q}{m}+c} \delta(q + mc - \sqrt{m^2 c^2 - 2q_z k}) \quad (5.42)$$

$$\times \left( \frac{D_{-1}}{|q|} + D_0 \right) (1 + \ln(\frac{D_{-1}}{|q|} + D_0) A_1 q) + h.o.T.$$

$$= -4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \int dq \frac{1}{\frac{q}{m}+c} \delta(|q| + mc - \sqrt{m^2 c^2 - 2q_z k})$$

$$\times (D_{-1}q) + h.o.T.$$

$$= -4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z \frac{m}{\sqrt{m^2 c^2 - 2q_z k}} \left( D_{-1}(\sqrt{m^2 c^2 - 2q_z k} - mc) + h.o.T. \right) \quad (5.43)$$

$$= -4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 \int_{-a}^0 dq_z D_{-1} \left( \frac{k}{mc^2} \right) q_z + h.o.T.$$

$$= -4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2 D_{-1} \frac{k}{2mc^2} a^2 + h.o.T.$$

As shown in (5.18)  $a$  is given by  $(k - k_f)$  and we find:

$$b(k) = -4\sqrt{2}\Gamma\pi^{\frac{3}{2}}e^2\tilde{c}^2D_{-1}\frac{k_f}{2mc^2}(k - k_f)^2 \quad (5.44)$$

Inserting  $D_{-1}$  as given in (5.37), the expression above gives:

$$b(k) = -\frac{k_f}{2m^3c^3}(k - k_f)^2 \quad (5.45)$$

which means

$$B = -\frac{k_f}{m^3c^3} \quad (5.46)$$

### 5.4.3. Discussion

Using the asymptotic behaviour for the one-particle energies as given in (5.24) and the assumptions as made in (5.32), we have shown, that equations (5.25) and (5.30) are solved self-consistently. There is only one assumption left, we have to consider. This is  $d = 1$ , where  $\alpha = 0$ .

For  $d(k, q)$  we now have  $d = 1 + A_1q + B(|k + q| - k_f)2 - b(k - k_f)$ . This obviously is not constantly equal one. In the following section we will investigate the case, where  $\alpha(\infty)$  is shifted from  $\alpha(0)$ , such that for the relevant region of integration  $d$  indeed equals one. In the next chapter we will then take a look on equations (5.25) and the second line of (5.30), when  $d$  is non constant.

## 5.5. A Self Consistent Solution

We now have to show, that our ansatz is indeed self-consistent.

Here we investigate the form of  $d_{k,q}$ , as is needed for the calculation of the integral in (5.30):

$$d_{k,q} = b_{k+q} - b_k + b_q = 1 \quad (5.47)$$

as long as

$$\alpha_{k,q}(\infty) = 0 \quad (5.48)$$

where  $\alpha$  has the extensive form:

$$\begin{aligned} \alpha_{k,q}(\infty) &= \epsilon_{k+q}(\infty) - \epsilon_k(\infty) + \omega_q(\infty) \\ &= \epsilon_{k+q}(0) - \frac{B(|k+q|-k_f)^2}{E_1|k+q-k_f|} - \epsilon_k(0) + \frac{B(k-k_f)^2}{E_1|k-k_f|} + \omega_q - \frac{1+A_1q}{\frac{D-1}{q}+D_0+D_1q} \end{aligned} \quad (5.49)$$



The first equation (5.47) is easily seen to yield

$$d_{k,q} = B(|k + q| - k_f)^2 - B(k - k_f)^2 + 1 + A_1q \quad (5.50)$$

$$= B|k + q|^2 - Bk^2 - 2Bk_f(|k + q| - k) + 1 + A_1q$$

Using (5.49) we can now transform this expression to:

$$2mB(-cq + \frac{B}{E_1}(|k + q| - k) + \frac{1}{D_{-1}}q) - 2Bk_f(|k + q| - k) + 1 + A_1q = \quad (5.51)$$

$$1 - 2mcBq + \frac{2mB}{D_{-1}}q + A_1q + \frac{2mB^2}{E_1}(|k + q| - k) - 2Bk_f(|k + q| - k)$$

Choosing  $E_1 = \frac{mB}{k_f}$  this means:

$$d_{k,q} = 1 - (2mcB + \frac{2mB}{D_{-1}} + A_1)q \quad (5.52)$$

In order for this expression to be one, we can put:

$$A_1 = -2mB(c + \frac{1}{D_{-1}}) \quad (5.53)$$

This not only proves the self consistency of our assumptions, but just as well leaves us with a possibility to calculate the constants.

### 5.5.1. Discussion

We have shown in this section, that - with a shifted asymptotic behaviour - we can indeed find a  $d_{k,q}$ , which self-consistently solves equations (5.30). Looking at the solution of this section, however, one sees the following:

$$\epsilon_k(\infty) = \frac{1}{2m}k^2 - \frac{k_f}{m}(k - k_f) \quad (5.54)$$

This leads to a fermi velocity, given by:

$$v_f = \frac{d\epsilon_{k_f}}{dk} = 0 \quad (5.55)$$

The fermi velocity vanishes, which cannot be justified physically. Hence, we do not continue on this way to find a self-consistent solution. In the next chapter we turn to a non-constant  $d_{k,q}$ .



## 6. General equations for the shift of the asymptotic behaviour

### 6.1. General Remarks and Outline

In this chapter we will continue evaluating the integrals in (5.25) and (5.30) for the more general case, where  $d_{k,q}$  is a function of  $k, q$  and not necessarily constant for all those values of  $k, q$ , where  $\alpha_{k,q} = 0$ . Hence, we start with expressions (5.29) and (5.30):

$$b(q) = 2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2q\sqrt{\ell}\int_B\delta(\alpha_q(k))(n_{k+q}-n_k)\ell^{-\frac{1}{2}d_q^2(k)} \\ \times \prod_{i\neq j}(\frac{1}{4}(\ell_i+\ell_j)+\frac{1}{2}\sqrt{\ell_i\ell_j})^{\frac{1}{2}b_ib_j}\ell_1^{\frac{1}{2}b_1^2}\ell_2^{\frac{1}{2}b_2^2}\ell_3^{\frac{1}{2}b_3^2}d^3k \quad (6.1)$$

and

$$b(k) = -2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2q\sqrt{\ell}\int_B\delta(\alpha_k(q))(1-n_{k+q})\ell^{-\frac{1}{2}d_k^2(q)} \\ \times \prod_{i\neq j}(\frac{1}{4}(\ell_i+\ell_j)+\frac{1}{2}\sqrt{\ell_i\ell_j})^{\frac{1}{2}b_ib_j}\ell_1^{\frac{1}{2}b_1^2}\ell_2^{\frac{1}{2}b_2^2}\ell_3^{\frac{1}{2}b_3^2}d^3q \quad (6.2)$$

To continue we set:

$$F(k, q) := \prod_{i\neq j}(\frac{1}{4}(\ell_i+\ell_j)+\frac{1}{2}\sqrt{\ell_i\ell_j})^{\frac{1}{2}b_ib_j}\ell_1^{\frac{1}{2}b_1^2}\ell_2^{\frac{1}{2}b_2^2}\ell_3^{\frac{1}{2}b_3^2} \quad (6.3)$$

$$C := 2\sqrt{2}\Gamma\sqrt{\pi}e^2\tilde{c}^2$$

We now have:

$$b(q) = Cq\sqrt{\ell}\int_B\delta(\alpha_q(k))(n_{k+q}-n_k)F_q(k)\ell^{-\frac{1}{2}d_q^2(k)}d^3k \quad (6.4)$$

$$b(k) = -C\sqrt{\ell}\int_B\delta(\alpha_k(q))(1-n_{k+q})qF_k(q)\ell^{-\frac{1}{2}d_k^2(q)}d^3q \quad (6.5)$$

To evaluate an integral of this type we will proceed similar to the way given in appendix A. First we investigate the behaviour of  $d_{k,q}^2$  and show, that is given by an expression of the form  $1 + g_{k,q}$  where the latter is strictly positive. Then we use

$$\lim_{\ell \rightarrow \infty} \left( \int_B \delta(\alpha_{q,k})(n_{k+q} - n_k) F_q(k) e^{-g_q(k) \ln \ell} d^3 k \right) \quad (6.6)$$

$$= \sqrt{\pi} \int_B \delta(\alpha_q(k)) \delta(g_q(k)) (n_{k+q} - n_k) F_q(k) d^3 k$$

to continue the transformation of our integrals (6.4), (6.5). We start the next section by investigating  $g(q,k)$ .

## 6.2. Calculating the general expression

### 6.2.1. Investigation of the exponential

We will use the results of the last chapter to find the Ansatz for  $g(q, k)$

$$b(k) = B|k - k_f|(k - k_f), \quad (6.7)$$

as B is negative, this is negative for  $k > k_f$  and positive for  $k < k_f$ . and we put

$$b(q) = 1 + Aq^2 \quad (6.8)$$

Note: The Ansatz in the last line is not exactly the one of the last chapter. At this point the choice is for mathematical convenience only.

As in (6.1)  $d_{k,q}$  is given by:

$$d_{k,q} = 1 + aq^2 + B ||k + q| - k_f| (|k + q| - k_f) - B|k - k_f|(k - k_f) \quad (6.9)$$

We want to investigate expressions containing terms of the type:  $e^{-\frac{1}{2}d_{k,q}^2 \ln \ell}$ . To do so we need to find those values of  $q$  and  $k$ , for which  $g(q, k) := d^2(q, k) - 1$  equals zero. We also have to show, that  $g(k, q) \geq 0$  for all values of  $q$  and  $k$ . We are only interested in the “relevant” values of  $q$  and  $k$ , i.e. those values, where  $\alpha(q, k, \infty) \approx 0$ .

We start by investigating  $g_q(k)$ , as is needed for the evaluation of equation (6.4). For the relevant region of integration in (6.4) we have:  $|k + q| < k_f < k$ .

$$g_q(k) = d_q^2(k) - 1 = 2Aq^2 - 2B(|k + q| - k_f)^2 - 2B(k - k_f)^2 \quad (6.10)$$

For fixed  $q$  the  $k$  values relevant in the integration (6.4) are defined by:

$$\begin{aligned}\alpha = 0 : \quad & \frac{k_z q}{m} + \frac{q^2}{2m} + cq = 0 \\ |k + q| &= \sqrt{k^2 + 2k_z q + q^2} \\ &= \sqrt{k^2 - 2mcq} \approx k - \frac{mc}{k}q\end{aligned}\tag{6.11}$$

We find for  $g_q(k)$  :

$$\begin{aligned}2Aq^2 - 2B \left( k - k_f - \frac{mcq}{k} - \frac{m^2 c^2 q^2}{2k^3} \right)^2 - 2B (k - k_f)^2 \\ = 2Aq^2 + 4B(k - k_f) \left( \frac{mcq}{k} \right) - 2B \frac{m^2 c^2 q^2}{k^2_f} - 4B(k - k_f)^2 \\ + 2 \left( A - B \frac{m^2 c^2}{k^2} \right) q^2 + 4B(k - k_f) \frac{mc}{k} q\end{aligned}\tag{6.12}$$

Terms of higher order in  $q$  and  $(k - k_f)$  are neglected here, as well as in subsequent calculations.

We set  $\Delta k := (k - k_f)$  and use  $k \approx k_f$ :

$$2 \left( A - B \frac{m^2 c^2}{k_f^2} \right) q^2 + 4B(\Delta k) \frac{mc}{k_f} q - 4B(\Delta k)^2\tag{6.13}$$

Note:  $B < 0$ . We write for (6.13):

$$-4B \left( (\Delta k) - \frac{1}{2} \frac{mc}{k_f} q \right)^2 + (2A - B \frac{m^2 c^2}{k_f^2}) q^2\tag{6.14}$$

This function of  $\Delta k$  is a parabel with minimum at  $\left( \frac{1}{2} \frac{mc}{k_f} q / (2A - B \frac{m^2 c^2}{k_f^2}) q^2 \right)$ . To have  $g_q(k)$  to equal zero at the minimum, we choose:

$$A = \frac{1}{2} B \frac{m^2 c^2}{k_f^2}\tag{6.15}$$

Then we find the desired:

$$g_q(k) = -4B \left( (\Delta k) - \frac{1}{2} \frac{mc}{k_f} q \right)^2\tag{6.16}$$

For the evaluation of (6.5) we consider:

$$g_k(q) = 2Aq^2 + B(|k + q| - k_f)^2 - B(k - k_f)^2 \quad (6.17)$$

Here we are interested in the values of  $q$ , for wich:

$$\alpha_k(q) = \frac{kq_z}{m} + \frac{q^2}{2m} + cq = 0 \text{ i.e. } q_z < 0 : \quad q = -mc + \sqrt{m^2c^2 - 2kq_z} \approx -\frac{k}{mc}q_z \quad (6.18)$$

then we find:

$$|k + q| \approx k + q_z \approx k - \frac{mc}{k_f}q \quad (6.19)$$

We now continue with:

$$\begin{aligned} g_k(q) &= 2Aq^2 + B((k - k_f) + q_z)^2 - B(k - k_f)^2 \\ &= 2Bq_z^2 + 2Bq_z(k - k_f) \end{aligned} \quad (6.20)$$

where for the last line we used (6.15) and (6.18). We have found a parabel with maximum at:  $(-\frac{1}{2}\Delta k / -\frac{1}{2}B(\Delta k)^2)$ . As we will show later, this means  $g_k(q)$  equals zero at the boundary of the integration values of the integral in (6.5).

### 6.2.2. Evaluation of the Integrals

We now calculate  $b(q)$  and  $b(k)$  using (6.4) and (6.5), respectively. We change coordinates in the first equation

$(k_x, k_y, k_z) \rightarrow (k, k_z, \phi)$  and perform the integration over the azimuthal symmetry. In the following we closely follow the calculation as given in 5.3.1. Note: the function  $F$  is not equivalent to the one used in equation (5.12).

$$\begin{aligned} b(q) &= 2\pi Cq\sqrt{\ell} \int_{B^2} kdkdk_z (n_{k+q} - n_k) F_q(k, k_z) \\ &\quad \times e^{-\frac{1}{2}\ln \ell - \frac{1}{2}g_q(k)\ln \ell} \delta\left(\frac{q^2}{2m} - \frac{k_zq}{m} + cq\right) \\ &= 2\pi Cq \int_{k_f}^{\sqrt{k_f^2 - q^2 - 2k_zq}} kdk \int_0^{k_f} dk_z \delta\left(\frac{q^2}{2m} - \frac{k_zq}{m} + cq\right) F(k, k_z) e^{-\frac{1}{2}g_q(k)\ln \ell} \\ &= 2\pi Cm \int_{k_f}^{\sqrt{k_f^2 + 2mcq}} k_f dk F(k, k_z = -\frac{q}{2} - mc) e^{2B\left((\Delta k) - \frac{1}{2}\frac{mc}{k_f}q\right)^2 \ln \ell} \end{aligned} \quad (6.21)$$

We use similar arguments as in chapter 4 and in appendix A to find this expression to equal:

$$b(q) = 2\pi^{\frac{3}{2}} C m k_f \frac{1}{\sqrt{-2B}} F_q(k = k_f + \frac{1}{2} \frac{mc}{k_f} q, k_z = -\frac{q}{2} - mc) \frac{1}{\sqrt{\ln \ell}} \quad (6.22)$$

We now calculate  $b(k)$ . We use the constant  $a = (k - k_f)$  as calculated in (5.18) and we use the approximation:  $q = -mc + \sqrt{m^2 c^2 - 2k q_z} = -\frac{k}{mc} q_z$ . In addition we use  $k \approx k_f$ .

$$\begin{aligned} b(k) &= -2\pi C \sqrt{\ell} \int_{B^2} dq_z dq q^2 \delta(\alpha_k(q)) F_k(q, q_z) e^{-\frac{1}{2} \ln \ell - \frac{1}{2} g_k(q) \ln \ell} \\ &= -2\pi C \int_{-a}^0 dq_z \int dq q^2 \frac{1}{\frac{q}{m} + c} \delta(q + mc - \sqrt{m^2 c^2 - 2k q_z}) F_k(q) e^{-\frac{1}{2} g_k(q) \ln \ell} \\ &= -2\pi C \int_{-a}^0 dq_z \frac{k_f^2}{m^2 c^3} q_z^2 F_k(q = -\frac{k}{mc} q_z, q_z) e^{-(B q_z^2 + B q_z (k - k_f)) \ln \ell} \end{aligned} \quad (6.23)$$

At both boundaries, we now have an integral of the type:  $\int_0^\infty e^{-const \cdot q_z \ln \ell} dq_z$ . For  $\ell \rightarrow \infty$  this is readily seen to yield  $\frac{1}{const \cdot \ln \ell}$ . We now find:

$$\begin{aligned} b(k) &= -2\pi C \frac{1}{(-B)(k - k_f)} \\ &\times \left[ \left\{ \frac{k_f^2}{m^2 c^3} q_z^2 F_k(q = -\frac{k}{mc} q_z, q_z) \right\}_{q_z=0} \right. \\ &\left. + \frac{k_f^2}{m^2 c^3} (k - k_f)^2 F_k(q = -\frac{k}{mc} q_z, q_z = (k - k_f)) \right] \frac{1}{\ln \ell} \end{aligned} \quad (6.24)$$

### 6.3. Logarithmic Counter Terms

To continue evaluating (6.22) and (6.24), we first need to get rid of the logarithmic factors. This can be done by adding an additional term to our Ansatz for the flow of the one particle energies:

$$\omega_q(\ell) = \omega_q(\infty) + \frac{b_q}{2\sqrt{\ell + \ell_0(q)}} + \frac{e_q}{2\sqrt{\ell + \tilde{\ell}_0(q)} \ln(\ell + \tilde{\ell}_0(q))} \quad (6.25)$$

$$\epsilon_k(\ell) = \epsilon_k(\infty) + \frac{b_k}{2\sqrt{\ell + \ell_\epsilon(k)}} + \frac{e_k}{2\sqrt{\ell + \tilde{\ell}_\epsilon(k)} \ln(\ell + \tilde{\ell}_\epsilon(k))} \quad (6.26)$$

As before we have  $\alpha_{k,q}(\infty) := \epsilon_{k+q}(\infty) - \epsilon_k(\infty) + \omega_q(\infty)$  and we define:  
 $d_{k,q} := b_{k+q} - b_k + b_q$ , in addition we also set:  $e_{k,q} := e_{k+q} - e_k + e_q$ .

In the same way as in chapter 5, see equations (5.25) and (5.30), we have to solve equations for  $b(q)$  and  $b(k)$  containing expressions of the kind  $e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'}$ . We start by calculating

$$\begin{aligned}
 & \int_0^\ell \alpha_{k,q}^2(\ell') d\ell' \\
 &= \ell \alpha^2 + 2\alpha d_{k,q} \sqrt{\ell} + 2\alpha e_{k,q} \frac{\sqrt{\ell}}{\ln \ell} \\
 & - 2\alpha \sum_i b_i \sqrt{\ell_i} - 2\alpha \sum_i e_i \frac{\sqrt{\tilde{\ell}_i}}{\ln \tilde{\ell}_i} + \frac{d_{k,q}^2}{4} \ln \ell + \frac{1}{2} d_{k,q} e_{k,q} \ln \ln \ell \\
 & + f(k, q)
 \end{aligned} \tag{6.27}$$

where we set:  $\ell_1 = \ell_{k+q}$ ,  $\ell_2 = \ell_k$ ,  $\ell_3 = \ell_q$

and  $b_1 = b_{k+q}$ ,  $b_2 = -b_k$ ,  $b_3 = b_q$ , with analogous definitions for the  $e_i$  and  $\tilde{\ell}_i$ .

We neglected terms of order  $\int \frac{1}{\sqrt{\ell' \ln^2 \ell'}} d\ell'$  and terms like

$\frac{1}{\ln \ell}$ ; and we used:  $\ell + \ell_i \approx \ell$ , as well as  $\ell + \tilde{\ell}_i \approx \ell$ .

As the second line of (6.27) does not contribute ( $\alpha \approx 0$ ),  $f(k, q)$  includes all the effects of the  $\ell_i$  and  $\tilde{\ell}_i$ . If one neglects the dependency on  $\tilde{\ell}_i$  altogether we have:

$$e^{-2f(k,q)} = F(k, q) \tag{6.28}$$

where  $F$  is the function as defined in (6.3).

We now have:

$$\begin{aligned}
 & -2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell' = \\
 & -2\ell \left( \alpha_{k,q} + \frac{d_{k,q}}{\sqrt{\ell}} + \frac{e_{k,q}}{\sqrt{\ell \ln \ell}} \right)^2 \\
 & + 2d_{k,q}^2 + O\left(\frac{1}{\ln^2 \ell}\right) - \frac{d_{k,q}^2}{2} \ln \ell - d_{k,q} e_{k,q} \ln \ln \ell - 2f(k, q)
 \end{aligned} \tag{6.29}$$

We insert expression (6.29) into the equations, which determine the  $b(q)$  and  $b(k)$ , i.e. (5.25) and (5.30). We use (6.28)



$$\begin{aligned}
 b(q) &= -8\Gamma e^2 \tilde{c}^2 q \ell^{\frac{3}{2}} \int_B \left( \alpha_q(k, \infty) + \frac{d_q(k)}{2\sqrt{\ell}} + \frac{e_q(k)}{2\sqrt{\ell} \ln \ell} \right) (n_{k+q} - n_k) \\
 &\quad \times e^{-\frac{1}{2} d_q^2(k) \ln \ell} (\ln \ell)^{-d_q(k) e_q(k)} F_q(k) e^{-2\ell \left( \alpha_q(k, \infty) + \frac{d_q(k)}{\sqrt{\ell}} + \frac{e_q(k)}{\sqrt{\ell} \ln \ell} \right)^2} d^3 k
 \end{aligned} \tag{6.30}$$

$$\begin{aligned}
 b(k) &= 8\Gamma e^2 \tilde{c}^2 q \ell^{\frac{3}{2}} \int_B \left( \alpha_k(q, \infty) + \frac{d_k(q)}{2\sqrt{\ell}} + \frac{e_k(q)}{2\sqrt{\ell} \ln \ell} \right) (1 - n_{k+q}) \\
 &\quad \times e^{-\frac{1}{2} d_k^2(q) \ln \ell} (\ln \ell)^{-d_k(q) e_k(q)} F_k(q) e^{-2\ell \left( \alpha_k(q, \infty) + \frac{d_k(q)}{\sqrt{\ell}} + \frac{e_k(q)}{\sqrt{\ell} \ln \ell} \right)^2} d^3 q
 \end{aligned}$$

Once again using as transformation as in chapter 4 and appendix A, these equations become:

$$\begin{aligned}
 b(q) &= 2\sqrt{2}\Gamma \sqrt{\pi} e^2 \tilde{c}^2 q \sqrt{\ell} \int_B \left( d_q(k) + \frac{e_q(k)}{\ln \ell} \right) (n_{k+q} - n_k) \\
 &\quad \times e^{-\frac{1}{2} d_q^2(k) \ln \ell} (\ln \ell)^{-d_q(k) e_q(k)} F_q(k) \delta(\alpha_q(k)) d^3 k
 \end{aligned} \tag{6.31}$$

$$\begin{aligned}
 b(k) &= -2\sqrt{2}\Gamma \pi e^2 \tilde{c}^2 q \ell \int_B \left( d_k(q) + \frac{e_k(q)}{\ln \ell} \right) (1 - n_{k+q}) \\
 &\quad \times e^{-\frac{1}{2} d_k^2(q) \ln \ell} (\ln \ell)^{-d_k(q) e_k(q)} F_k(q) \delta(\alpha_k(q)) d^3 q
 \end{aligned}$$

We follow the same way as in (6.2.2) to transform these expressions to:

$$\begin{aligned}
 b(q) &= 2\pi^{\frac{3}{2}} C m k_f \frac{1}{\sqrt{-2B}} F_q(k = k_f + \frac{1}{2} \frac{mc}{k_f} q, k_z = -\frac{q}{2} - mc) \\
 &\quad \times (\ln \ell)^{-\frac{1}{2} - e_q(k=k_f + \frac{1}{2} \frac{mc}{k_f} q, k_z = -\frac{q}{2} - mc)} \\
 b(k) &= -2\pi C \frac{1}{(-B)(k-k_f)} \\
 &\quad \times \left[ \left\{ \frac{k_f^2}{m^2 c^3} q_z^2 F_k(q = -\frac{k}{mc} q_z, q_z) \right\}_{q_z=0} + \frac{k_f^2}{m^2 c^3} (k - k_f)^2 F_k(q = -\frac{k}{mc} q_z, q_z = (k - k_f)) \right] \\
 &\quad \times (\ln \ell)^{-1 - e_k(q = -\frac{k}{mc} q_z, q_z = (k - k_f))}
 \end{aligned} \tag{6.32}$$

$F_q(k, k_z)$  and  $F_k(q, q_z)$  can be seen as one function of  $F(q, k, |k + q|)$ . In addition we choose the  $e_q = 1$  and  $e_k = -\text{sgn}(k - k_f)\frac{1}{4}$ . We insert our assumptions  $b(q) = 1$  and  $b(k) = B(k - k_f)^2$  into (6.32), which we then rewrite:

$$\begin{aligned}
 1 &= 2\pi^{\frac{3}{2}} C m k_f \frac{1}{\sqrt{-2B}} F(q, k = k_f + \frac{1}{2} \frac{mc}{k_f} q, |k + q| = k_f - \frac{1}{2} \frac{mc}{k_f} q) \\
 B^2(k - k_f)^2 &= 2\pi C \frac{1}{c} \left[ \left\{ q^2 F_k(q = \frac{k_f}{mc}(k - k_f), k, |k + q| = k) \right\}_{q=0} \right. \\
 &\quad \left. + \frac{k_f^2}{m^2 c^3} (k - k_f)^2 F_k(q = \frac{k_f}{mc}(k - k_f), k, |k + q| = k_f) \right]
 \end{aligned} \tag{6.33}$$

These two equations can be seen as fundamental set of equations for the investigation of the shift of the asymptotic behaviour or more general for the dependency of the one-particle energies on  $\ell$  before the onset of the asymptotic behaviour.

### 6.3.1. Discussion

In this chapter we have continued our investigation of equations (5.25) and (5.30). It is necessary to have  $d_{k,q}^2 > 1$  for all values of  $q$  and  $k$  which belong to resonances and  $d_{k,q}^2$  to equal one, at least at one “relevant” point in every region of integration of the integrals in (5.29) and (5.30). Here we have assumed the most general form possible. This has led to an additional  $\delta$  function, as well as terms logarithmic in  $\ell$ , when evaluating equations (6.4) and (6.5). By adding terms of higher order in  $\ln \ell$  to the asymptotic flow of the one-particle energies, we were able to find counter terms and refine the leading order of our asymptotic behaviour.

We then found equations, which can be used to determine the  $q$  and  $k$  dependency of the shift in the asymptotic behaviour.

Taking a look at (6.33) it is easily seen, that  $F(q, k, |k + q|)$  has to depend, not only on  $q$ , but on  $k, |k + q|$ , as well. As  $F$  is given by (6.3), this means, that the  $\ell_\epsilon$  have to contribute. As was seen in (5.32), this does not happen, if they behave no more singular, than poles at the fermi surface. Hence, we are led to assume a behaviour of the  $\ell_\epsilon(k)$  like:

$$\ell_\epsilon(k) = e^{\frac{1}{(k - k_f)^n}} \tag{6.34}$$

## 7. Transformation of the One-Particle Operators

### 7.1. General Remarks

In this chapter we calculate the transformation of the one-particle electron operators. The transformation is similar to the one of the phonon-operators, investigated by Wegner and Ragwitz in [7]. They used their results to calculate the phonon-correlation function.

In 2.2 we gave the general behaviour of any arbitrary operator under the  $\ell$ -induced transformation. One can consider the formalism of Hamiltonian Flow Equations as an implicit, continuous transformation of the basis, where for  $\ell \rightarrow \infty$  an eigenbasis of the Hamiltonian is found. For every  $\ell$  any operator has to be presented in the basis corresponding to this very  $\ell$ .

According to (2.7) the change of the electronic creation operators  $c_k^+$  are governed by:

$$\frac{dc_k^+(\ell)}{d\ell} = [\eta(\ell), c_k^+(\ell)] \quad (7.1)$$

where  $\eta(\ell)$  is given by (3.16):

$$\sum_{k,q} (\alpha_{k,q}(\ell) M_{k,q}(\ell) a_{-q}^+ - \alpha_{k+q,-q}(\ell) M_{k+q,-q}(\ell) a_q) c_{k+q}^+ c_k \quad (7.2)$$

### 7.2. Differential Equations for the Electron Operators

#### 7.2.1. Electron-Creation-Operators

For the form of the electronic creation operators under the  $\ell$  induced transformation we make the following Ansatz:

$$c_k^+(\ell) = u_k^+(\ell) c_k^+ + \sum_q u_{k,q}^+(\ell) a_{-q}^+ c_{k+q}^+ + \sum_q u_{k,q}(\ell) a_q c_{k+q}^+ \quad (7.3)$$

Here  $u_k^+(\ell)$ ,  $u_{k,q}^+(\ell)$  and  $u_{k,q}(\ell)$  are  $\ell$  dependent functions, with the starting values:  $u_k^+(0) = 1$ ,  $u_{k,q}^+(0) = u_{k,q}(0) = 0$ . In (7.3) higher order terms, i.e. normal ordered multiples of creation and annihilation operators are neglected.

To find the differential equations as induced by (7.1) and (7.2), we need to calculate the following commutators:

$$\left[ \sum_{k',q} M_{k',q} \alpha_{k',q} a_{-q}^+ c_{k'+q}^+ c_{k'}, c_k^+ \right] = \sum_q M_{k,q} \alpha_{k,q} a_{-q}^+ c_{k+q}^+ \quad (7.4)$$

$$\left[ - \sum_{k',q} M_{k'+q,-q} \alpha_{k'+q,-q} a_q c_{k'+q}^+ c_{k'}, c_k^+ \right] = \sum_q -M_{k+q,-q} \alpha_{k+q,-q} a_q c_{k+q}^+ \quad (7.5)$$

$$\left[ \sum_{k',q'} M_{k',q'} \alpha_{k',q'} a_{-q'}^+ c_{k'+q'}^+ c_{k'}, a_{-q}^+ c_{k+q}^+ \right] = \sum_{q'} M_{k+q,q'} \alpha_{k+q,q'} : a_{-q}^+ a_{-q'}^+ : c_{k+q+q'}^+ \quad (7.6)$$

$$\begin{aligned} & \left[ - \sum_{k',q'} M_{k'+q',-q'} \alpha_{k'+q',-q'} a_{q'} c_{k'+q'}^+ c_{k'}, a_{-q}^+ c_{k+q}^+ \right] \\ &= -M_{k,q} \alpha_{k,q} (1 - n_{k+q}) c_k^+ - M_{k,q} \alpha_{k,q} n_{-q} c_k^+ \\ & - \sum_{k'} M_{k'-q,q} \alpha_{k'-q,q} : c_{k'-q}^+ c_{k'}^+ c_{k+q}^+ : - \sum_{q'} M_{k+q-q',-q'} \alpha_{k+q-q',-q'} : a_{-q}^+ a_{q'}^+ : c_{k+q+q'}^+ \end{aligned} \quad (7.7)$$

$$\begin{aligned} & \left[ \sum_{k',q'} M_{k',q'} \alpha_{k',q'} a_{-q'}^+ c_{k'+q'}^+ c_{k'}, a_q c_{k+q}^+ \right] \\ &= M_{k+q,-q} \alpha_{k+q,-q} n_{k+q} c_k^+ + M_{k+q,-q} \alpha_{k+q,-q} n_q c_k^+ \end{aligned} \quad (7.8)$$

$$\begin{aligned} & - \sum_{k'} M_{k',-q} \alpha_{k',-q} : c_{k+q}^+ c_{k'-q}^+ c_{k'}^+ : + \sum_{q'} M_{k+q,q'} \alpha_{k+q,q'} : a_{-q}^+ a_{q'}^+ : c_{k+q+q'}^+ \\ & \left[ - \sum_{k',q'} M_{k'+q',-q'} \alpha_{k'+q',-q'} a_{q'} c_{k'+q'}^+ c_{k'}, a_q c_{k+q}^+ \right] \end{aligned} \quad (7.9)$$

$$= \sum_{q'} -M_{k+q+q',-q'} \alpha_{k+q+q',-q'} a_q a_{q'} c_{k+q+q'}^+$$

This yields the following set of differential equations:

$$\frac{du_k^+(\ell)}{d\ell} = -\sum_q M_{k,q}(\ell)\alpha_{k,q}(\ell)(1-n_{k+q})u_{k,q}^+(\ell) - \sum_q M_{k,q}(\ell)\alpha_{k,q}(\ell)n_{-q}u_{k,q}^+(\ell) \quad (7.10)$$

$$+ \sum_q M_{k+q,-q}(\ell)\alpha_{k+q,-q}(\ell)n_{k+q}u_{k,q}(\ell) + \sum_q M_{k+q,-q}(\ell)\alpha_{k+q,-q}(\ell)n_q u_{k,q}(\ell)$$

$$\frac{du_{k,q}^+(\ell)}{d\ell} = +M_{k,q}(\ell)\alpha_{k,q}(\ell)u_k^+(\ell) \quad (7.11)$$

$$\frac{du_{k,q}(\ell)}{d\ell} = -M_{k+q,-q}(\ell)\alpha_{k+q,-q}(\ell)u_k^+(\ell) \quad (7.12)$$

We work in the regime  $T = 0$ , where the expectation value to find a phonon is zero and, hence, we have  $n_q = 0$ .

### 7.2.2. Electron-Annihilation Operators

Similarly the Ansatz for the transformation of the electron-annihilation operators is given by:

$$c_k(\ell) = u_k^{+*}(\ell)c_k + \sum_q u_{k,-q}^{+*}(\ell)a_{-q}^+c_{k-q} + \sum_q u_{k,-q}^{+*}(\ell)a_q c_{k-q} \quad (7.13)$$

and one finds a set of differential equations equivalent to: (7.10)-(7.12).

## 7.3. Solving the Differential Equations

We now solve the differential equations governing the transformation of the electron-creation-operators. First we insert equations (7.11) and (7.12) in (7.10), which gives:

$$\begin{aligned} \frac{du_k^+(\ell)}{d\ell} = & -\sum_q M_{k,q}(\ell)\alpha_{k,q}(\ell)(1-n_{k+q}) \int_0^\ell M_{k,q}(\ell')\alpha_{k,q}(\ell')u_k^+(\ell')d\ell' \\ & - \sum_q M_{k+q,-q}(\ell)\alpha_{k,q}(\ell)n_{k+q} \int_0^\ell M_{k+q,-q}(\ell')\alpha_{k+q,-q}(\ell')u_k^+(\ell')d\ell' \end{aligned} \quad (7.14)$$

In addition equations (4.6)-(4.9) hold, of course.

Just as in our discussion in section 5.1, we find, that for  $k > k_f$  only the first term of this integro-differential equation is of importance, i.e. the second term decays exponentially, whereas for  $k < k_f$  only the second term has to be considered. Here we explicitly solve equation (7.14) for  $k > k_f$  only. The case  $k < k_f$  can be handled in exactly the same way.

We know the asymptotic behaviour of  $\alpha_{k,q}(\ell)$  to be of the form:

$$\alpha_{k,q}(\ell) = \alpha_{k,q}(\infty) + \frac{b(k+q)-b(k)+b(q)}{2\sqrt{\ell+\ell_0}}$$

We use this form, and not the more refined one as given in (5.24), for reasons of clearness, only. The calculation for the more refined case is done in a completely analogous way.

Note: for the following we assume  $b(k+q) - b(k) + b(q) = 1$  for all values of  $k$  and  $q$  within the region of integration with:  $\alpha_k(q, \infty) = 0$ . For a more detailed discussion on this assumption see section 5.4 and 6.

Using (4.6), we have:

$$\begin{aligned} \frac{du_k^+(\ell)}{d\ell} = & -\tilde{c}^2 \sum_q \int_0^\ell u_k^+(\ell') e^{-\int_0^{\ell'} \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell''+\ell_0}} \right)^2 d\ell''} \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell'+\ell_0}} \right) d\ell' \\ & \times e^{-\int_0^\ell \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell''+\ell_0}} \right)^2 d\ell''} \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell+\ell_0}} \right) (1 - n_{k+q}) \end{aligned} \quad (7.15)$$

where as before  $|M_q|^2 = \tilde{c}^2 q$

In the asymptotic regime, we assume  $u_k^+(\ell)$  to show an algebraic behaviour of the kind  $\tilde{b}_k(\ell + \tilde{\ell}_0(q))^{-\gamma}$ . For the following we can neglect  $\ell_0(q)$  as  $\ell \gg \tilde{\ell}_0$  and we divide both left and right hand side of equation (7.15) by  $\tilde{b}_k$ . We replace the summation over  $k$  by an integration.

$$\begin{aligned} & -\Gamma \tilde{c}^2 \int_B \int_0^\ell \ell'^{-\gamma} q e^{-\int_0^{\ell'} \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell''+\ell_0}} \right)^2 d\ell''} e^{-\int_0^\ell \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell''+\ell_0}} \right)^2 d\ell''} \\ & \times \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell'+\ell_0}} \right) d\ell' \left( \alpha_k(q, \infty) + \frac{1}{2\sqrt{\ell+\ell_0}} \right) (1 - n_{k+q}) d^3q \end{aligned} \quad (7.16)$$

We calculate the exponent in this equation:

$$\begin{aligned}
 & - \int_0^{\ell'} \left( \alpha_{k,q}(\infty) + \frac{1}{2\sqrt{\ell'' + \ell_0}} \right)^2 d\ell'' - \int_0^{\ell} \left( \alpha_{k,q}(\infty) + \frac{1}{2\sqrt{\ell^* + \ell_0}} \right)^2 d\ell^* \\
 & = -\alpha_{k,q}^2(\ell + \ell') - 2\alpha_{k,q}(\sqrt{\ell + \ell_0} + \sqrt{\ell' + \ell_0}) + 4\alpha_{k,q}\sqrt{\ell_0} \\
 & \quad - \frac{1}{4} \ln(\ell + \ell_0) - \frac{1}{4} \ln(\ell' + \ell_0) + \frac{1}{2} \ln(\ell_0) \\
 & = -(\ell + \ell') \left( \alpha_{k,q} + \frac{\sqrt{\ell + \ell_0} + \sqrt{\ell' + \ell_0}}{\ell + \ell'} \right)^2 + 1 + \frac{2\ell_0}{\ell + \ell'} + \frac{2\sqrt{\ell + \ell_0}\sqrt{\ell' + \ell_0}}{\ell + \ell'} \\
 & \quad + 4\alpha_{k,q}\sqrt{\ell_0} - \frac{1}{4} \ln(\ell + \ell_0) - \frac{1}{4} \ln(\ell' + \ell_0) + \frac{1}{2} \ln(\ell_0)
 \end{aligned} \tag{7.17}$$

As the relevant values of  $q$  are given by:  $\alpha_k(q, \infty) \approx 0$  we can neglect the term  $2\alpha_k(q)\sqrt{\ell_0}$ .

We insert this expression in (7.16):

$$\begin{aligned}
 & = -\Gamma e \tilde{c}^2 \int_0^{\ell} \int_k \ell'^{-\gamma} q \ell_0^{\frac{1}{2}} \left( \alpha_{k,q}(\infty) + \frac{1}{2\sqrt{\ell' + \ell_0}} \right) \left( \alpha_{k,q}(\infty) + \frac{1}{2\sqrt{\ell + \ell_0}} \right) \\
 & \quad \ell^{-\frac{1}{4}} \ell'^{-\frac{1}{4}} e^{-(\ell + \ell')} \left( \alpha_{k,q} + \frac{\sqrt{\ell + \ell_0} + \sqrt{\ell' + \ell_0}}{\ell + \ell'} \right)^2 e^{\frac{2\ell_0}{\ell + \ell'} + \frac{2\sqrt{\ell + \ell_0}\sqrt{\ell' + \ell_0}}{\ell + \ell'}} (1 - n_{k+q}) d^3 q d\ell'
 \end{aligned} \tag{7.18}$$

For  $\ell \rightarrow \infty$ , this expression is transformed as in 4.23. We find:

$$\begin{aligned}
 & = -\Gamma \pi^{\frac{1}{2}} e \tilde{c}^2 \int_0^{\ell} \int_B \ell'^{-\gamma} \delta(\alpha_k(q)) q \ell_0^{\frac{1}{2}} \\
 & \quad \times \left( -\frac{\sqrt{\ell + \ell_0} + \sqrt{\ell' + \ell_0}}{\ell + \ell'} + \frac{1}{2\sqrt{\ell' + \ell_0}} \right) \left( -\frac{\sqrt{\ell + \ell_0} + \sqrt{\ell' + \ell_0}}{\ell + \ell'} + \frac{1}{2\sqrt{\ell + \ell_0}} \right) \\
 & \quad \times \ell^{-\frac{1}{4}} \ell'^{-\frac{1}{4}} \frac{1}{\sqrt{\ell + \ell'}} e^{\frac{2\ell_0}{\ell + \ell'} + \frac{2\sqrt{\ell + \ell_0}\sqrt{\ell' + \ell_0}}{\ell + \ell'}} (1 - n_{k+q}) d^3 q d\ell'
 \end{aligned} \tag{7.19}$$

We are in the asymptotic regime and choose  $\ell$  such that  $\ln \ell \gg \ell_0$ ;<sup>1</sup> in leading order

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<sup>1</sup>As we have  $\ell_0(q) \sim \frac{1}{q^2}$ , this is only true for the larger part of the region of integration. We neglect effects due to the region of integration, where  $q > \frac{1}{\sqrt{\ln \ell}}$

expression (7.19) is equivalent to:

$$\begin{aligned}
 & -2\Gamma\pi^{\frac{3}{2}}e\tilde{c}^2 \int_{\ln \ell}^{\ell} \int_{B^2} \ell'^{-\gamma} \delta(\alpha_k(q)) q^2 \ell_0^{\frac{1}{2}} \\
 & \times \left( -\frac{\sqrt{\ell+\ell_0}+\sqrt{\ell'+\ell_0}}{\ell+\ell'} + \frac{1}{2\sqrt{\ell'+\ell_0}} \right) \left( -\frac{\sqrt{\ell+\ell_0}+\sqrt{\ell'+\ell_0}}{\ell+\ell'} + \frac{1}{2\sqrt{\ell+\ell_0}} \right) \\
 & \times \ell^{-\frac{1}{4}} \ell'^{-\frac{1}{4}} \frac{1}{\sqrt{\ell+\ell'}} e^{\frac{2\ell_0}{\ell+\ell'} + \frac{2\sqrt{\ell+\ell_0}\sqrt{\ell'+\ell_0}}{\ell+\ell'}} (1 - n_{k+q}) dq dq_z d\ell'
 \end{aligned} \tag{7.20}$$

We can now use  $\ell + \ell_0 \approx \ell$  and  $\ell' + \ell_0 \approx \ell'$ , to find:

$$\begin{aligned}
 & -2\Gamma\pi^{\frac{3}{2}}e\tilde{c}^2 \int_{\ln \ell}^{\ell} \int_{B^2} \ell'^{-\gamma} \delta(\alpha_k(q)) q^2 \ell_0^{\frac{1}{2}} \\
 & \times \left( -\frac{\sqrt{\ell}+\sqrt{\ell'}}{\ell+\ell'} + \frac{1}{2\sqrt{\ell'}} \right) \left( -\frac{\sqrt{\ell}+\sqrt{\ell'}}{\ell+\ell'} + \frac{1}{2\sqrt{\ell}} \right) \ell^{-\frac{1}{4}} \ell'^{-\frac{1}{4}} \frac{1}{\sqrt{\ell+\ell'}} e^{\frac{2\sqrt{\ell}\sqrt{\ell'}}{\ell+\ell'}} (1 - n_{k+q}) dq dq_z d\ell'
 \end{aligned} \tag{7.21}$$

We exchange the integrals to find:

$$\begin{aligned}
 & -2\Gamma\pi^{\frac{3}{2}}e\tilde{c}^2 \int_{B^2} \delta(\alpha_k(q)) q^2 \ell_0^{\frac{1}{2}} (1 - n_{k+q}) dq dq_z \\
 & \times \int_{\ln \ell}^{\ell} \ell'^{-\gamma} \left( -\frac{\sqrt{\ell}+\sqrt{\ell'}}{\ell+\ell'} + \frac{1}{2\sqrt{\ell'}} \right) \left( -\frac{\sqrt{\ell}+\sqrt{\ell'}}{\ell+\ell'} + \frac{1}{2\sqrt{\ell}} \right) \ell^{-\frac{1}{4}} \ell'^{-\frac{1}{4}} \frac{1}{\sqrt{\ell+\ell'}} e^{\frac{2\sqrt{\ell}\sqrt{\ell'}}{\ell+\ell'}} d\ell'
 \end{aligned} \tag{7.22}$$

We now use the equivalent to the second line of (5.30):

$$b(k) = -4\sqrt{2}\Gamma\sqrt{\pi}^{\frac{3}{2}}e^2\tilde{c}^2 \int_{B^2} q^2 \delta(\alpha_q(k)) \ell_0^{\frac{1}{2}} (1 - n_{k+q}) dq dq_z \tag{7.23}$$

and find:

$$\begin{aligned}
 \frac{du_k^+(\ell)}{d\ell} &= \frac{b(k)}{2\sqrt{2}} \exp(-1) \int_{\ln \ell}^{\ell} \ell'^{-\gamma} \left( -\frac{1}{\sqrt{\ell}} \frac{1+\sqrt{\frac{\ell'}{\ell}}}{1+\frac{\ell'}{\ell}} + \frac{1}{2\sqrt{\ell'}} \right) \left( -\frac{1}{\sqrt{\ell}} \frac{1+\sqrt{\frac{\ell'}{\ell}}}{1+\frac{\ell'}{\ell}} + \frac{1}{2\sqrt{\ell}} \right) \\
 & \times \ell^{-\frac{1}{4}} \ell'^{-\frac{1}{4}} \frac{1}{\sqrt{\ell}} \frac{1}{\sqrt{1+\frac{\ell'}{\ell}}} \exp\left(\frac{2\sqrt{\frac{\ell'}{\ell}}}{1+\frac{\ell'}{\ell}}\right) d\ell'
 \end{aligned} \tag{7.24}$$



We set:  $x = \frac{\ell'}{\ell}$  and the expression becomes:

$$\begin{aligned} & \frac{b(k)}{2\sqrt{2}} \exp(-1) \ell^{-1-\gamma} \int_0^1 \left[ x^{-\gamma-\frac{1}{4}} \left( \frac{1+\sqrt{x}}{1+x} \right)^2 \frac{1}{\sqrt{1+x}} \exp\left(\frac{2\sqrt{x}}{1+x}\right) \right. \\ & \quad \left. - \frac{1}{2} x^{-\gamma-\frac{1}{4}} \frac{1+\sqrt{x}}{1+x} \frac{1}{\sqrt{1+x}} \exp\left(\frac{2\sqrt{x}}{1+x}\right) \right. \\ & \quad \left. - \frac{1}{2} x^{-\gamma-\frac{3}{4}} \frac{1+\sqrt{x}}{1+x} \frac{1}{\sqrt{1+x}} \exp\left(\frac{2\sqrt{x}}{1+x}\right) + \frac{1}{4} x^{-\gamma-\frac{3}{4}} \frac{1}{\sqrt{1+x}} \exp\left(\frac{2\sqrt{x}}{1+x}\right) \right] dx \end{aligned} \quad (7.25)$$

As we are interested in the asymptotic behaviour for  $\ell \rightarrow \infty$  we could replace  $\frac{\ln \ell}{\ell}$  by 0 at the lower boundary of our integral. We can now insert  $u_k^+(\ell)$  into the left hand side of (7.24),  $b(k) = -\frac{k_f^3}{2m^3c^3}(k - k_f)^2$  from equation (5.45) into the right hand side and write  $Int$  instead of the integral. We then find:

$$-\gamma \ell^{-1-\gamma} = - \left( \frac{1}{2\sqrt{2}e} \frac{k_f^3}{2m^3c^3} (k - k_f)^2 \cdot Int \right) \ell^{-\gamma-1} \quad (7.26)$$

The  $\ell$ -dependency of the left and right-hand side of this equation is the same and we can use this equation to determine  $\gamma$ :

$$\gamma = \left( \frac{1}{2\sqrt{2}e} \frac{k_f^3}{2m^3c^3} \cdot Int(\gamma) \right) (k - k_f)^2 \quad (7.27)$$

where we have written  $Int(\gamma)$  to show, that the integral itself does depend on  $\gamma$ . For small values of  $\gamma$  this dependency, however, is relatively small, as compared to the  $(k - k_f)^2$ -dependency. Numerical calculations yield:

$$\begin{aligned} \gamma = 0 : & \quad Int = -0.129 \\ \gamma = 0.01 : & \quad Int = -0.240 \\ \gamma = 0.05 : & \quad Int = -0.349 \end{aligned}$$

This means, we find:

$$\gamma \sim -(k - k_f)^2 \quad (7.28)$$

### 7.3.1. Discussion

One would actually expect to find (7.28) without a minus sign. Then the spreading out of the electronic one-particle operators would depend on the distance of these electrons to the fermi surface, with the spreading out becoming slower and slower as  $k$  approaches the fermi surface.

In this form, however, (7.28) shows a contradiction. We assumed  $u_k^+(\ell)$  to depend on  $\ell$  like  $\ell^{-\gamma}$ . (7.28) describes a growing  $u_k^+(\ell)$ , which is clearly not possible.

Hence, the transformation of the electron-one-particle operators is not given by an algebraic form.



## 8. Conclusion

In this thesis we have investigated the electron-phonon-Hamiltonian (3.1) using the method of Hamiltonian Flow Equations. Starting point of our analysis was the fundamental set of coupled integro-differential equations, as found by Wegner and Lenz [5]. This set of equations governs the flow of the interaction constants and the one particle energies under the  $\ell$ -induced transformation. Very little experience exists how to handle these equations. Therefore, this work has partly the character of a mathematical study rather than attempting to calculate physical quantities. Several mathematical results have been obtained.

The renormalization of the energies is given by the difference of the one particle energies at the start of the transformation ( $\ell = 0$ ) and its end ( $\ell \rightarrow \infty$ ). In a first step we have proved that the inclusion of the electronic flow into the set of differential equations does not alter the behaviour of the phononic flow in the asymptotic regime. For large values of  $\ell$  the flow of the one particle energies is given by

$$\omega_q + \frac{b(q)}{2\sqrt{\ell}} \quad , \quad \epsilon_k + \frac{b(k)}{2\sqrt{\ell}}$$

for the phonons and electrons respectively. The  $b(q)$  and  $b(k)$  remain to be determined, from the differential form of the flow equations. Other algebraic behaviours, i.e. a flow of the type  $\frac{const}{\ell^\gamma}$ , with  $\gamma \neq \frac{1}{2}$  are not possible. Using this result, it was seen that the interaction constants do decay as  $\ell \rightarrow \infty$ ; most of them exponentially, only for those values of  $q$  and  $k$  for which we have resonances, i.e.

$\alpha_{k,q} := \epsilon_{k+q} - \epsilon_k + \omega_q \approx 0$  the decay is given by

$$M_{k,q}(\ell) \sim \ell^{-\frac{1}{4}}.$$

In a second step we have investigated the functions  $b(q)$  and  $b(k)$ . One is led to shift the asymptotic behaviour in the same way as in the work of Wegner and Ragwitz [7]. We chose the form

$$\omega_q + \frac{b(q)}{2\sqrt{\ell + \ell_0(q)}} \quad , \quad \epsilon_k + \frac{b(k)}{2\sqrt{\ell + \ell_\epsilon(k)}}$$

for the flow of the one particle energies.

The  $\ell_0$  is found to equal the one Wegner and Ragwitz found for the case where the electronic flow is neglected. The  $\ell_\epsilon(k)$  remain undetermined at this point.

This shifted asymptotic behaviour yields  $b(q) = 1$  and  $b(k) = -\frac{k_f}{m^3 c^3} (k - k_f)^2$ . A result

like this is necessary, as the fundamental set of equations leads to a contradiction, if  $d_{k,q} := b(k+q) - b(k) + b(q) \neq 1$  for values of  $q$  and  $k$  which belong to resonances.

In chapter 5 we searched for a solution with  $d_{k,q}$  equal to one on the line of resonances. Such a solution could be found; the physical use, however, seems doubtful, as the fermi velocity would vanish.

In the subsequent chapter we have investigated an Ansatz using a non constant  $d_{k,q}$ . This has led to terms logarithmic in  $\ell$ , violating the self-consistency of the Ansatz. To refine a  $\frac{const}{2\sqrt{\ell}}$  asymptotic behaviour in the leading term, we introduced an additional term  $\frac{const}{2\sqrt{\ell} \ln \ell}$  for the asymptotic behaviour of the electronic and phononic energies. We found an equation for the shift of the asymptotic behaviour. This equation has been discussed, but remains to be fully solved. Using the additional term in the flow of the one-particle energies as a hint, we changed - in appendix B - the asymptotic behaviour of the electrons to

$$\epsilon_k(\ell) = \epsilon_k(\infty) + \frac{1}{2\sqrt{\ell + \ell_\epsilon} \ln(\ell + \ell_\epsilon)}$$

The leading term of the phononic flow was refound, as well as the absolut value of the leading terms of the electronic energies. The final equation of chapter 6 suggested a singular behaviour of  $\ell_\epsilon(k)$  at the fermi surface.

$$\ell_\epsilon(k) = e^{\frac{1}{(k-k_f)^n}} \quad n > 0$$

A similar behaviour for the  $\ell_\epsilon(k)$  was assumed for our investigations in appendix B. The renormalization of the electronic energies found in chapter 5:

$$\Delta\epsilon_k = \epsilon_k(\infty) - \epsilon_k(0) = \frac{-b(k)}{2\sqrt{\ell_\epsilon(k)}}$$

yielded the renormalization near the fermi surface:

$$\Delta\epsilon_k = const \cdot (k - k_f)^2 \cdot e^{-\frac{1}{(k-k_f)^2}}$$

for the constellation discussed in chapter 6. The renormalization drops to zero exponentially as  $k$  approaches the fermi surface. Comparing this result to a standard text-book (e.g. [9]) shows a large discrepancy. This, however, is explained easily: We have not included the attractive electron-electron-interaction of the transformed Hamiltonian in our mathematical study. On the other hand this interaction is the major source of the renormalization of the electrons.

In the last chapter of this thesis, chapter 7, we have calculated the transformation of the electronic one-particle operators

$$c_k^+(\ell) := u_k^+(\ell)c_k^+ + \sum_q u_{k,q}^+(\ell)a_{-q}^+c_{k+q}^+ + \sum_q u_{k,q}(\ell)a_q c_{k+q}^+.$$

---

The assumption of an algebraic decay of  $u_k^+$  lead to a contradiction. Hence, we got an indication, that the decay is not purely algebraically.

In principle the results of the electronic one particle transformation can be used to calculate the electronic correlation function. This, as well as a solution of the fundamental equations of chapter 6, requires considerable additional effort.



## A. Mathematical proof

In this appendix we give a proof for the calculations of the type as given in chapter 4. I.e. we show:

for  $\ell \rightarrow \infty$

$$\int_{B^3} d^3 q \alpha_{k,q}(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \quad (\text{A.1})$$

behaves like

$$\frac{\text{const}}{\ell} \int f_k(q) \ell^{(b_{k+q}-b_k+b_q)^2} \delta(\alpha_k(q)) d^3 q + O\left(\frac{\ln \ell}{\sqrt{\ell^3}}\right) \ell^{d_{min}^2}$$

and

$$\int_{B^3} d^3 k \alpha_{k,q}(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \quad (\text{A.2})$$

behaves like

$$\frac{\text{const}}{\ell} |M_q|^2 \int f_k(q) \ell^{(b_{k+q}-b_k+b_q)^2} \delta(\alpha_q(k)) d^3 q + O\left(\frac{\ln \ell}{\sqrt{\ell^3}}\right) \ell^{d_{min}^2}$$

where

$$\alpha_{k,q}(\ell) = \epsilon_{k+q}(\ell) - \epsilon_k(\ell) + \omega_q(\ell) \quad (\text{A.3})$$

depends only on  $\ell, k, q, |k+q|$

$$d_{k,q} = b_{k+q} - b_k + b_q$$

$d_{min}$  is the minimum of this function within the region of integration and:

$$\begin{aligned} \epsilon_k(\ell) &= \epsilon_k(\infty) + \frac{b_k}{2\sqrt{\ell}} \\ \omega_q(\ell) &= \omega_q(\infty) + \frac{b_q}{2\sqrt{\ell}}, \end{aligned} \quad (\text{A.4})$$

as long as  $\ell > \ell_0$  and  $\alpha_{k,q}(\ell)$  is a smooth and bounded function for all  $\ell < \ell_0$   
 $f_k(q) = d_k(q) |M(q)|^2 e^{-2\alpha_k(q, \ell^*)} \ell_0^{\frac{1}{2} d_k^2(q)} e^{2d_k^2(q)}$  and

$f_q(k) = d_q(k)e^{-2\alpha_q(k, \ell^{**})} \ell_0^{\frac{1}{2}d_q^2(k)} e^{2d_q^2(k)}$  are smooth functions.  $(\ell^*)$   $(\ell^{**})$  are fixed values between 0 and  $\ell_0$ .

$B^3$  is the first Brillouin zone and  $|M_q|^2 = \tilde{c}^2 q$ . N.B. in the following we will use  $B$  to denote the bound of the Brillouin zone and  $B^2$  to denote the Brillouin zone, when the variables are transformed to cylindrical coordinates and the integral over the azimuth is performed. Further we set:  $\tilde{c} = 1$ .

The first integral is needed to find the derivative of the flow of the electronic one particle energies, the second for the flow of the phononic one particle energies.

Here we explicitly prove only the behaviour of the integrals in (A.1) and (A.2) under the assumption (A.4). Other algebraic decays of the one particle energies would lead to similar equations and the behaviour of the integrals (A.1) and (A.2) is found and proven in a similar way, as well. In the following we will first give the proof for (A.1), (A.2) will be proven in the second section.

### A.1. The Algebraic Decay of the Integral governing the Electronic Flow

To show more clearly which of the variables are integrated over, we rewrite the integral of the first line of (A.2) as:

$$\int_{B^3} d^3q \alpha_k(q, \ell) |q| e^{-2 \int_0^\ell (\alpha_k(q, \ell'))^2 d\ell'} \quad (\text{A.5})$$

with

$$\alpha_k(q, \ell) = \alpha_k(q, \infty) + \frac{d_k(q)}{2\sqrt{\ell}}$$

in the asymptotic regime.

We defined  $b(k+q) - b_k + b(q) =: d_k(q)$ .

To deal with the integral above, we make the following

**Assumptions:**

- a)  $\alpha_k(q, \infty) \in C^\infty$  and  $|\alpha_k(q, \infty)|$  bounded by  $Q$ .
- b)  $\epsilon(k, \infty)$  and  $\omega(q, \infty)$  are strictly monotonuos increasing functions of  $k$  resp.  $q$ .
- c)  $\left| \frac{\partial^2 \epsilon}{\partial k^2} \right|_{k=k_0} > \left| \frac{\partial^2 \omega}{\partial q^2} \right|_{q=q_0} \quad \forall k_0, q_0$ .
- d) The  $b(k)$  and  $b(q)$  are  $\in C^\infty$  and  $d_k(q)$  is bounded by  $D$ .
- e) The  $\ell$ -dependency of  $\alpha$  is given by (A.4) for all values of  $\ell$ :  $\ell > \ell_0$ .
- f) For all  $\ell$   $\alpha_k(q, \ell)$  depends only on  $|k|$ ,  $|q|$  and  $|k+q|$ .<sup>1</sup>

As  $k$  is fixed in the integral (A.5) we can transform to cylindrical coordinates, i.e.  $(q_1, q_2, q_3) \rightarrow (q_\perp, q_z, \phi)$ , where the  $z$ -axis,  $(0, q_z, 0)$  is chosen parallel to  $\vec{k}$ . We can

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<sup>1</sup>Not all of these assumptions are necessary for the following proof. Some of them are made for convenience only. From a physical point they do make sense.



now perform the integration over the angle:

$$\int_{B^3} d^3q \alpha_k(q, \ell) |q| e^{-2 \int_0^\ell (\alpha_k(q, \ell'))^2 d\ell'} \quad (\text{A.6})$$

$$= 2\pi \int_{B^2} dq_z dq_\perp \quad q_\perp q \alpha_k(q_z, q_\perp, \ell) e^{-2 \int_0^\ell (\alpha_k(q_z, q_\perp, \ell'))^2 d\ell'} \quad (\text{A.7})$$

here  $B^2$  denotes the transformed Brillouin zone of  $q_z, q_\perp$  and  $q = |q|$ .

### Lemma 1

The set of all elements in the  $q_z, q_\perp$  plane such that  $\alpha_k(q_z, q_\perp, \infty) = 0$ ,  $S := \{(q_\perp, q_z) | \alpha_k(q_\perp, q_z, \infty) = 0\}$ , is either a regular one dimensional compact manifold, or  $S = \{(0, 0)\}$

#### Proof:

a) The set  $S := \{(q_\perp, q_z) | \alpha_k(q_\perp, q_z, \infty) = 0\}$  is compact: As  $B^2$  is bounded,  $S$  is bounded as well. As  $B^2$  is closed and  $\alpha_k(q_\perp, q_z, \infty)$  is continuous,  $S$  is closed. Thus  $S$  is compact.

b) We show, that  $S = \{(0, 0)\}$  or  $S$  does not contain isolated points. A point in  $S$  can only be isolated, if it is a local minimum or maximum of  $\alpha_k(q_\perp, q_z, \infty)$ ,

i.e.  $\frac{\partial \alpha_k(q_\perp, q_z, \infty)}{\partial q_\perp} = \frac{\partial \alpha_k(q_\perp, q_z, \infty)}{\partial q_z} = 0$ . This is seen easily using the theorem on implicit functions.

To investigate whether isolated points exist we take a look at the first derivatives. As  $\frac{\partial \alpha}{\partial q_\perp} = q_\perp \left( \frac{\partial \epsilon}{\partial x} \frac{1}{(k+q_z)^2 + q_\perp^2} + \frac{\partial \omega}{\partial x} \frac{1}{\sqrt{q_z^2 + p^2}} \right) \forall q_\perp \neq 0$ , (see Assumption b))

we only have to consider points in  $S \cap \{(q_z, 0)\}$ . At those points, we have

$\alpha_k(q_z, 0, \infty) = \epsilon(k + q_z) + \omega(|q_z|) - \epsilon(k)$ , where  $k$  is parallel to  $q_z$ .

Without loss of generality we assume  $k > 0$  and we find

$$\frac{\partial \alpha}{\partial q_z} = \frac{\partial \epsilon}{\partial x} \Big|_{x=|k+q_z|} \text{sign}(k + q_z) + \frac{\partial \omega}{\partial x} \Big|_{x=|q_z|} \text{sign}(q_z).$$

Hence, this derivative can only be zero on the interval  $q_z \in [-k, \dots, 0]$ .

We have  $\alpha_k(q_z = 0, 0, \ell) = 0$ . At this point ( $q_z = 0$ )  $\alpha(k, q)$  is not differentiable, because  $\omega(q_z, \ell = 0)$  is a function of  $|q_z|$ . Instead we simply use right hand and left hand derivatives.

The right hand derivative is always positive.

$\frac{\partial \alpha}{\partial q_z}$  is monotonously increasing on  $[0, \infty[$ . If the left hand derivative at  $q_z = 0$  is  $\leq 0$ , then we have a local minimum at this point  $(0, 0)$ . It follows immediately, that  $S = \{(0, 0)\}$ . If, on the other hand, the left hand derivative at  $q_z = 0$  is  $> 0$ , we can use  $\alpha_k(0, B, \infty) \gg 0$  to show, that there is a  $q_z^* < 0$  such that  $\alpha_k(0, q_z, \infty) < 0$  on  $]q_z^*, 0[$  and  $\alpha_k(q_z^*, 0, \infty) = 0$ . As the derivative at this point is different from 0, there are no isolated points in  $S$ .

c) We show that  $S$  is connected. As  $\alpha_k(q_{||0}, q_\perp, \infty)$  is strictly monotonous increasing with  $|q_\perp|$  and  $\alpha_k(q_z, 0, \infty) \leq 0 \forall q_z \in [q_z^*, \dots, 0]$  and bigger than 0 outside of this interval,  $S$  is connected (unless cut into parts by the region of integration).

The above proves Lemma 1

For the following we restrict ourselves to the case, where  $S \neq \{(0, 0)\}$

We now show, that we can restrict ourselves to a small surrounding of this one-dimensional-manifold in evaluating our integral.

**Lemma 2**

Let  $\delta > 0$ , then we have for  $\ell \rightarrow \infty$ :

$$2\pi \int_{B^2} dq_z dq_\perp \quad q_\perp q \alpha_k(q_z, q_\perp, \ell) e^{-2 \int_0^\ell (\alpha_k(q_z, q_\perp, \ell'))^2 d\ell'} = \quad (\text{A.8})$$

$$2\pi \int_{|\alpha_k(q_z, q_\perp, \infty)| \leq \delta} dq_z dq_\perp \quad q_\perp q \alpha_k(q_z, q_\perp, \ell) e^{-2 \int_0^\ell (\alpha_k(q_z, q_\perp, \ell'))^2 d\ell'} + O(e^{-\ell}) \quad (\text{A.9})$$

**Proof:**

Let  $(q_z, q_\perp)$  be outside the region of integration of the second integral (i.e.  $|\alpha_k(q_\perp, q_z, \infty)| > \delta$ , than we can choose  $\ell_1 > \ell_0$  such that  $\frac{d}{2\sqrt{\ell}} < \frac{\delta}{2} \quad \forall \ell > \ell_1$ , meaning that

$|\alpha_k(q_\perp, q_z, \infty) + \frac{d_k(q_z)}{2\sqrt{\ell}}| > \frac{\delta}{2}$ . Note that the region of integration is defined by  $\alpha_k(\cdot, \cdot, \infty) < \delta$  and in the integrand we have  $\alpha_k(\cdot, \cdot, \ell'), \ell' < \ell$ .

We have:

$$\begin{aligned} & \left| \int_{B^2 \setminus \{(q_\perp, q_z), |\alpha_k(q_z, q_\perp, \infty)| \leq \delta\}} dq_z dq_\perp \quad q_\perp q \alpha_k(q_z, q_\perp, \ell) e^{-2 \int_0^\ell (\alpha_k(q_z, q_\perp, \ell'))^2 d\ell'} \right| \\ & < |B^2| Q q_B e^{-\delta(\ell - \ell_1)} \end{aligned} \quad (\text{A.10})$$

wher  $Q$  is the upper bound of  $\alpha_{k,q}(\infty)$  (A.1) and  $q_B$  is the upper bound for  $q$  in  $B^3$   
This proves Lemma 2.

Using our assumptions on the asymptotic behaviour of  $\alpha_k(q_z, q_\perp, \ell)$  for  $\ell \gg \ell_0$ , we can perform:

**Calculation 1**

$$\begin{aligned} & \int_0^\ell \alpha_k(q_z, q_\perp, \ell')^2 d\ell' = \int_0^{\ell_0} [\alpha_k(q_z, q_\perp, \ell')^2 - \alpha_k(q_z, q_\perp, \infty)^2] d\ell' \\ & + \int_0^\ell \alpha_k(q_z, q_\perp, \infty)^2 d\ell' + \int_{\ell_0}^\ell \frac{d_k(q_z, q_\perp)}{\sqrt{\ell'}} \alpha_k(q_z, q_\perp, \infty) d\ell' + \int_{\ell_0}^\ell \frac{d_k^2(q_z, q_\perp)}{4\ell'} \end{aligned} \quad (\text{A.11})$$

$$\begin{aligned}
 &= \alpha_k(q_z, q_\perp, \infty)^2 \ell + 2d_k(q_z, q_\perp) \alpha_k(q_z, q_\perp, \infty) \sqrt{\ell} + d_k^2(q_z, q_\perp) \frac{1}{4} \ln \ell \\
 &\quad - 2d_k(q_z, q_\perp) \alpha_k(q_z, q_\perp, \infty) \sqrt{\ell_0} - d_k^2(q_z, q_\perp) \frac{1}{4} \ln \ell_0
 \end{aligned} \tag{A.12}$$

$$+ [\alpha_k(q_z, q_\perp, \ell^*)^2 - \alpha_k(q_z, q_\perp, \infty)^2] \ell_0$$

here  $\ell^*$  is given by  $\int_0^{\ell_0} \alpha_k(q_z, q_\perp, \ell')^2 d\ell' = \alpha_k(q_z, q_\perp, \ell^*)^2 \ell_0$ , which is simply the mean value theorem of integration calculus.

This leads to:

$$\begin{aligned}
 &\exp \left( -2 \int_0^\ell \alpha_k(q_z, q_\perp, \ell')^2 d\ell' \right) \\
 &= \exp \left( -2\ell \left( \alpha_k(q_z, q_\perp, \infty) + \frac{d_k(q_z, q_\perp)}{\sqrt{\ell}} \right)^2 \right) \ell^{-\frac{1}{2}} d_k^2(q_z, q_\perp)
 \end{aligned} \tag{A.13}$$

$$\times \exp \left( -2[\alpha_k(q_z, q_\perp, \ell^*)^2 - \alpha_k(q_z, q_\perp, \infty)^2] \ell_0 \right)$$

$$\times \exp 2(2d_k(q_z, q_\perp) \alpha_k(q_z, q_\perp, \infty) \sqrt{\ell_0} + d_k^2(q_z, q_\perp) \frac{1}{4} \ln \ell_0) \exp 2d_k^2(q_z, q_\perp)$$

In the asymptotic regime the integral (A.5) takes the form:

$$\begin{aligned}
 &\int_B d^3q \alpha_k(q, \ell) |M(q)|^2 e^{-2 \int_0^\ell \alpha_k^2(q, \ell') d\ell'} \\
 &= 2\pi \int_{|\alpha_k(q_z, q_\perp)| \leq \delta} dq_z dq_\perp \quad q_\perp q \alpha_k(q_z, q_\perp, \ell) e^{-2 \int_0^\ell (\alpha_k(q_z, q_\perp, \ell'))^2 d\ell'} \\
 &= 2\pi \int_{|\alpha_k(q_z, q_\perp, \infty)| \leq \delta} dq_z dq_\perp \quad q_\perp q \left( \alpha_k(q_z, q_\perp, \infty) + \frac{d_k(q_z, q_\perp)}{2\sqrt{\ell}} \right) \\
 &\quad \times \exp \left( -2\ell \left( \alpha_k(q_z, q_\perp, \infty) + \frac{d_k(q_z, q_\perp)}{\sqrt{\ell}} \right)^2 \right) \ell^{-\frac{1}{2}} d_k^2(q_z, q_\perp) \\
 &\quad \times \exp \left( -2[\alpha_k(q_z, q_\perp, \ell^*)^2 - \alpha_k(q_z, q_\perp, \infty)^2] \ell_0 \right) \\
 &\quad \times \exp 2(2d_k(q_z, q_\perp) \alpha_k(q_z, q_\perp, \infty) \sqrt{\ell_0} + d_k^2(q_z, q_\perp) \frac{1}{4} \ln \ell_0) \exp 2d_k^2(q_z, q_\perp)
 \end{aligned} \tag{A.14}$$

We now introduce a transformation of variables.

Let the regular one-dimensional-manifold  $S$  of  $\alpha_k(q_\perp, q_z, \infty) = 0$  be given by:

$\phi : t \rightarrow \phi(t)$ , where we have chosen the parametrisation, such that:  $|\frac{d\phi(t)}{dt}| = 1$ .

As new coordinates, we introduce  $t$  along  $\alpha_k(\cdot, \cdot, \infty) = 0$  and  $u$  in the direction of the gradient of  $\alpha_k(\cdot, \cdot, \infty)$  by:  $q_z, q_\perp \rightarrow t, u$ . The transformation of our integral is then given according to [10]:

$$\int_{B^2} f(q_z, q_\perp) dq_z dq_\perp = \int_A f(g(t, u)) |J_g(t, u)| dt du \quad (\text{A.15})$$

The functional determinant  $J_g(t, u)$  is one, because we perform a orthonormal transformation.

For our integral we now have:

$$\begin{aligned} & 2\pi \int_{|\alpha_k(t, u, \infty)| \leq \delta} dt du q_\perp(t, u) q(t, u) \left( \alpha_k(t, u, \infty) + \frac{d_k(t, u)}{2\sqrt{\ell}} \right) \\ & \times \exp \left( -2\ell \left( \alpha_k(t, u, \infty) + \frac{d_k(t, u)}{\sqrt{\ell}} \right)^2 \right) \ell^{-\frac{1}{2} d_k^2(t, u)} \\ & \times \exp \left( -2[\alpha_k(t, u, \ell^*)^2 - \alpha_k(t, u, \infty)^2] \ell_0 \right) \\ & \times \exp 2(2d_k(t, u) \alpha_k(t, u, \infty) \sqrt{\ell_0} + d_k^2(t, u) \frac{1}{4} \ln \ell_0) \exp(2d_k^2(t, u)) \end{aligned} \quad (\text{A.16})$$

Note  $\alpha_k(t, 0, \infty) = 0 \forall t$  by definition.

We continue by investigating the integral over  $u$ .

As  $\vec{\nabla} \alpha_k(t, 0, \infty) = \frac{\partial \alpha}{\partial u}(t, 0, \infty) \neq 0$   $\alpha_k(t, u, \infty)$  is strictly monotonous in a surrounding of  $(t, 0)$ . Hence, we can now substitute  $u$  by  $\alpha_k(t, u, \infty) := z$ . As all functions are bounded within the region of integration, they will also be bounded after this substitution. We find:

$$\begin{aligned} & 2\pi \int_B dt \int_{z \leq \delta} dz q_\perp(t, z) q(t, z) \frac{1}{\frac{\partial \alpha}{\partial u}|_{(t, z)}} \left( z + \frac{d_k(t, z)}{2\sqrt{\ell}} \right) \\ & \times \exp \left( -2\ell \left( z + \frac{d_k(t, z)}{\sqrt{\ell}} \right)^2 \right) \ell^{-\frac{1}{2} d_k^2(t, z)} \exp \left( -2[\alpha_k(t, z, \ell^*)^2 - z^2] \ell_0 \right) \\ & \times \exp 2(2d_k(t, z) z \sqrt{\ell_0} + d_k^2(t, z) \frac{1}{4} \ln \ell_0) \exp 2d_k^2(t, z) \end{aligned} \quad (\text{A.17})$$

Note that the evaluation of  $\frac{1}{\frac{\partial \alpha}{\partial u}|_{(t, z)}}$  is by no means trivial, but the expression is well defined as function of  $t$  and  $z$ .

As a final substitution we now use  $z' = z + \frac{d_k(t, z)}{\sqrt{\ell}}$  and find for (A.17):

$$\begin{aligned}
 & 2\pi \int_B dt \int_{|z' - \frac{d_k(t, z)}{\sqrt{\ell}}| \leq \delta} dz' q_{\perp}(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}}) q(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}}) \frac{1}{1 + \frac{1}{\sqrt{\ell}} \frac{\partial d_k}{\partial z} |_{t, z(t, z')}} \\
 & \quad \times \frac{1}{\frac{\partial \alpha}{\partial u} |_{(t, z')}} (z' - \frac{d_k(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})}{2\sqrt{\ell}}) \exp(-2\ell z'^2) \\
 & \quad \times \ell^{-\frac{1}{2} d_k^2(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})} \exp\left(-2[\alpha_k(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}}, \ell^*)^2 - (z' - \frac{d_k(t, z)}{\sqrt{\ell}})^2] \ell_0\right) \\
 & \quad \times \exp\left(2(2d_k(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})(z' - \frac{d_k(t, z)}{\sqrt{\ell}})\sqrt{\ell_0} + d_k^2(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})\frac{1}{4} \ln \ell_0\right) \\
 & \quad \times \exp\left(2d_k^2(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})\right)
 \end{aligned} \tag{A.18}$$

All the functions under the integral sign are continuous and bounded. To continue we will use Lemma 3 and Lemma 4 to be proved later.

### Lemma 3

Let  $F_2(t, z)$ ,  $d_k(t, z)$ ,  $c_2(t, z)$  be bounded functions with bounded first derivatives, let  $\delta_1(t)$ ,  $\delta_2(t)$  be functions with  $\delta_1(t), \delta_2(t) > c^* > 0$  for all  $t$ , then we have:

$$\begin{aligned}
 & \left| \int_B dt \int_{-\delta_1(t)}^{\delta_2(t)} dz F_2(t, z - \frac{c_2(t, z)}{\sqrt{\ell}}) z \ell^{-\frac{1}{2} d_k^2(t, z - \frac{c_2(t, z)}{\sqrt{\ell}})} e^{-2z^2 \ell} \right| \\
 & \leq \text{const} \cdot \frac{\ln \ell}{\ell^{\frac{3}{2}}} \int_B \ell^{-\frac{1}{2} d_{min}^2(t)} dt
 \end{aligned} \tag{A.19}$$

where  $d_{min}$  is the minimum of  $d_k(t, z)$  on  $B \times [0, \delta_1]$ .

and

### Lemma 4

Let  $F_1(t, z)$ ,  $c_1(t, z)$  and  $d(t, z)$  be bounded functions with bounded derivatives, further let  $\delta_1(t), \delta_2(t) \geq a > 0 \forall t$  and  $B$  a one-dimensional compact connected region of integration, then we have:

$$\begin{aligned}
 & \int_B dt \int_{-\delta_1(t)}^{\delta_2(t)} dz F_1(t, z - \frac{c_1(t, z)}{\sqrt{\ell}}) \ell^{-\frac{1}{2} d_k^2(t, z - \frac{c_1(t, z)}{\sqrt{\ell}})} e^{-2z^2 \ell} \\
 & = \frac{1\sqrt{\pi}}{\sqrt{2\ell}} \int_B dt F_1(t) \ell^{-\frac{1}{2} d_k^2(t)} + O\left(\frac{\ln \ell}{\ell}\right) \int_B dt \ell^{-\frac{1}{2} d_{min}^2(t)}
 \end{aligned} \tag{A.20}$$

where we set  $F_1(t) := F_1(t, 0)$  and  $d_{min}^2$  is the minimum of  $d_k^2(t, z)$  on  $B \times [-\delta_1, \delta_2]$

Before giving the proof of Lemma 3 and 4 we finish our evaluation of (A.5) by first using Lemma 3 to find (A.21) and then Lemma 4 to reach (A.22):

$$\begin{aligned}
& \int_{B^3} d^3 q \alpha_k(q, \ell) |q| e^{-2 \int_0^\ell (\alpha_k(q, \ell'))^2 d\ell'} \\
& 2\pi \int_B dt \int_{(z' - \frac{d_k(t, z)}{\sqrt{\ell}}) \leq \delta} dz' q_\perp(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}}) q(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}}) \frac{1}{1 + \frac{1}{\sqrt{\ell}} \frac{\partial d_k}{\partial z} |_{t, z(t, z')}} \\
& \times \frac{1}{\frac{\partial \alpha}{\partial u} |_{t, u(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})}} \left( -\frac{d_k(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})}{2\sqrt{\ell}} \right) \exp -2\ell(z')^2 \\
& \times \ell^{-\frac{1}{2} d_k^2(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})} \exp -2[\alpha_k(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}}, \ell^*)^2 - (z' - \frac{d_k(t, z)}{\sqrt{\ell}})^2] \ell_0 \\
& \times \exp 2(2d_k(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})(z' - \frac{d_k(t, z)}{\sqrt{\ell}})\sqrt{\ell_0} + d_k^2(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})\frac{1}{4} \ln \ell_0) \\
& \times \exp 2d_k^2(t, z' - \frac{d_k(t, z)}{\sqrt{\ell}})
\end{aligned} \tag{A.21}$$

$$\begin{aligned}
& = -\frac{1}{\sqrt{2}} \pi^{\frac{3}{2}} \frac{1}{\ell} \int_B dt \quad q_\perp(t) q(t) \quad \frac{1}{\frac{\partial \alpha}{\partial u} |_{(t, 0)}} \quad \ell^{-\frac{1}{2} d_k^2(t)} \\
& \times \exp -2[\alpha_k(t, \ell^*)^2] \ell_0 \exp (d_k^2(t) \frac{1}{2} \ln \ell_0) \exp 2d_k^2(t)
\end{aligned} \tag{A.22}$$

Note: As Lemma 4 allows us to replace  $F_1(t, z - \frac{c}{\sqrt{\ell}})$  by  $F_1(t, 0)$  under the integral sign, we have  $\frac{1}{1 + \frac{1}{\sqrt{\ell}} \frac{\partial d_k}{\partial z}} \rightarrow 1$  and for the remaining integral we have  $z = z' + \frac{c}{\sqrt{\ell}} = 0$ . This is why, we can rewrite this expression and change the variables back to the original ones:

$$\begin{aligned}
& -\frac{1}{\sqrt{2}} \pi^{\frac{3}{2}} \int_B \int dt dz \delta(z) \quad \left[ q_\perp(t, z) q(t, z) \quad \frac{1}{\frac{\partial \alpha}{\partial u} |_{(t, z)}} \right. \\
& \times \exp -2[\alpha_k(t, z, \ell^*)^2] \ell_0 \exp (d_k^2(t, z) \frac{1}{2} \ln \ell_0) \exp 2d_k^2(t, z) \left. \right]
\end{aligned} \tag{A.23}$$

$$\begin{aligned}
& \stackrel{z \rightarrow u}{=} -\frac{1}{\sqrt{2}} \pi^{\frac{3}{2}} \int_B \int dt du \delta(u) \\
& \times [q_\perp(t, u) q(t, u) \exp -2[\alpha_k(t, z, \ell^*)^2] \ell_0 \exp (d_k^2(t, u) \frac{1}{2} \ln \ell_0) \exp 2d_k^2(t, u)]
\end{aligned} \tag{A.24}$$

$$\stackrel{t, u \rightarrow q_\perp, q_z}{=} -\frac{1}{\sqrt{2}}\pi^{\frac{3}{2}} \int_{B^2} dq_\perp dq_z \delta(\alpha(q_\perp, q_z)) \quad (\text{A.25})$$

$$\times [q_\perp q \exp -2[\alpha_k(q_\perp, q_z, \ell^*)^2] \ell_0 \exp(d_k^2(q_\perp, q_z) \frac{1}{2} \ln \ell_0) \exp 2d_k^2(q_\perp, q_z)]$$

This proves conjecture (A.1).

We now give the proofs of Lemma 3 and 4

**Proof** of Lemma 3:

Without loss of generality  $\delta_1(t) \leq \delta_2(t)$  for all  $t$ .

Integral (A.19) can be written as:

$$\begin{aligned} \int_B dt \int_0^{\delta_1(t)} \left[ F_2(t, z - \frac{c_2(t, z)}{\sqrt{\ell}}) \ell^{-\frac{1}{2}d_k^2(t, z - \frac{c_2(t, z)}{\sqrt{\ell}})} - F_2(t, -z - \frac{c_2(t, z)}{\sqrt{\ell}}) \ell^{-\frac{1}{2}d_k^2(t, -z - \frac{c_2(t, z)}{\sqrt{\ell}})} \right] z e^{-2\ell z^2} dz \\ + \int_B dt \int_{\delta_1(t)}^{\delta_2(t)} \left[ F_2(t, z - \frac{c_2(t, z)}{\sqrt{\ell}}) \ell^{-\frac{1}{2}d_k^2(t, z + \frac{c_2(t, z)}{\sqrt{\ell}})} \right] z e^{-2\ell z^2} dz \end{aligned} \quad (\text{A.26})$$

The second term obviously is smaller than  $const \cdot e^{-2\ell c^*2}$ . We continue with the first term (A.26):

$$\begin{aligned} \int_B dt \int_0^{\delta_1(t)} \left\{ \left[ \frac{\partial F_2}{\partial z} \Big|_{(t, z^*)} \left( \left( z - \frac{c_2(t, z)}{\sqrt{\ell}} \right) + \left( z + \frac{c_2(t, z)}{\sqrt{\ell}} \right) \right) \right] e^{-\frac{1}{2}d_k^2(t, z^*) \ln \ell} \right. \\ \left. + F_2(t, z^*) \left[ -\ln \ell \frac{\partial d_k}{\partial z} \Big|_{(t, z^*)} d_k(t, z^*) \ell^{-\frac{1}{2}d_k^2(t, z^*)} \left( \left( z - \frac{c_2(t, z)}{\sqrt{\ell}} \right) + \left( z + \frac{c_2(t, z)}{\sqrt{\ell}} \right) \right) \right] \right\} z e^{-2\ell z^2} dz \end{aligned} \quad (\text{A.27})$$

here for every  $z, z^* \in [0, z]$  such that

$$\frac{\partial(F_2 \cdot \ell^{-\frac{1}{2}d_k^2})}{\partial z} \Big|_{t, z^*} \cdot z = \left( F_2(t, z) \cdot \ell^{-\frac{1}{2}d_k^2(t, z)} - F_2(t, 0) \cdot \ell^{-\frac{1}{2}d_k^2(t, 0)} \right) \quad (\text{A.28})$$

Let  $d_{min}^2$  be the minimum of  $d_k^2(t, z)$  on  $B \times [0, \delta_1]$  and let  $M$  be the upper bound of  $\frac{\partial F_2}{\partial z}$  and  $F_2 \cdot \frac{\partial d_k}{\partial z} \cdot d_k$ , then the absolute value of the above is less than:

$$\begin{aligned} \int_B dt \int_0^{\delta_1(t)} 2M(1 + \ln \ell) \ell^{-\frac{1}{2}d_{min}^2} z^2 e^{-2\ell z^2} dz \\ \leq M(1 + \ln \ell) |B| \delta_1 \ell^{-\frac{1}{2}d_{min}^2} \frac{\sqrt{\pi}}{\ell^{\frac{3}{2}}} \end{aligned} \quad (\text{A.29})$$

q.e.d.

**Proof** of Lemma 4:

It is easily seen, that:

$$\frac{1\sqrt{\pi}}{\sqrt{2\ell}} \int_B dt F_1(t) \ell^{-\frac{1}{2}d_k^2(t)} = \int_B dt F_1(t) \ell^{-\frac{1}{2}d_k^2(t)} \int_{-\delta_1(t)}^{\delta_2(t)} e^{-2z^2\ell} dz + O(e^{-\ell}) \quad (\text{A.30})$$

thus we consider the difference of the left hand side and the first term of the right hand side of (A.20):

$$\begin{aligned} & \left| \int_B dt \int_{-\delta_1(t)}^{\delta_2(t)} \left( F_1(t, z - \frac{c_1(t,z)}{\sqrt{\ell}}) \ell^{-\frac{1}{2}d_k^2(t, z - \frac{c_1(t,z)}{\sqrt{\ell}})} - F_1(t) \ell^{-\frac{1}{2}d_k^2(t)} \right) e^{-2z^2\ell} dz \right| \\ &= \left| \int_B dt \int_{-\delta_1(t)}^{\delta_2(t)} \frac{\partial}{\partial z} \left\{ F_1(t, z) \ell^{-\frac{1}{2}d_k^2(t, z)} \right\} \Big|_{(t, z^*)} \left( z - \frac{c_1(t,z)}{\sqrt{\ell}} \right) e^{-2z^2\ell} dz \right| \\ &= \left| \int_B dt \int_{-\delta_1(t)}^{\delta_2(t)} \left( \frac{\partial F_1}{\partial z} \Big|_{(t, z^*)} - \ln \ell \frac{\partial d_k}{\partial z} \Big|_{(t, z^*)} d_k(t, z^*) F_1(t, z^*) \right) \ell^{-\frac{1}{2}d_k^2(t, z^*)} \left( z - \frac{c_1(t,z)}{\sqrt{\ell}} \right) e^{-2z^2\ell} dz \right| \end{aligned} \quad (\text{A.31})$$

Here  $z^*$  is given by the mean value theorem for differentiable functions:

$$\begin{aligned} & F_1(t, z - \frac{c_1(t,z)}{\sqrt{\ell}}) \ell^{-\frac{1}{2}d_k^2(t, z - \frac{c_1(t,z)}{\sqrt{\ell}})} e^{-2z^2\ell} - F_1(t) \ell^{-\frac{1}{2}d_k^2(t)} \\ &= \frac{\partial}{\partial z} \left\{ F_1(t, z) \ell^{-\frac{1}{2}d_k^2(t, z)} \right\} \Big|_{(t, z^*)} \left( z - \frac{c_1(t,z)}{\sqrt{\ell}} \right) \end{aligned} \quad (\text{A.32})$$

All the functions and their derivatives are bounded:  $|F_1(t, z)|$  by  $M_F$ ,  $|\frac{\partial F_1(t, z)}{\partial z}|$  by  $M_1$ ,  $|d_k(t, z)|$  by  $D$ ,  $|\frac{\partial d_k(t, z)}{\partial z}|$  by  $D_1$  and  $c_1(t, z)$  by  $M_c$ . Our integrand is then bounded by:

$$\int_B dt \int_{-\delta_1(t)}^{\delta_2(t)} (M_1 + \ln \ell D_1 D M_F) \ell^{-\frac{1}{2}d_k^2(t, z^*)} \left( |z| + \frac{M_c}{\sqrt{\ell}} \right) e^{-2z^2\ell} dz \quad (\text{A.33})$$

as  $d_k^2$  is bounded from below by  $d_{min}^2$  this expression is bounded by:

$$(M_1 + \ln \ell D_1 D M_F) (1 + M_c \frac{\sqrt{\pi}}{\sqrt{2}}) \frac{1}{\ell} \int_B \ell^{-\frac{1}{2}d_{min}^2} dt \quad (\text{A.34})$$

q.e.d.

## A.2. The Algebraic Decay of the Integral governing the Phononic Flow

For the derivatives of the  $\omega_q$ 's we have to study the behaviour of:

$$\int_B d^3 k \alpha_{k,q}(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \quad (\text{A.35})$$



In this case we assume the following:

**Assumptions 1'**

- a)  $\alpha_q(k, \infty) \in C^\infty$  and bounded by  $Q$ .
- b)  $\epsilon(k, \infty)$  and  $\frac{\partial \epsilon(|k|)}{\partial |k|}$  are strictly monotonuos increasing functions of  $k$ ,  $\omega(q, \infty)$  is strictly bigger than zero.
- c) The  $c(k)$  and  $a(q)$  are  $\in C^\infty$  and  $d_k(q)$  is bounded by  $D$ .
- d) For the moment, the asymptotic behaviour is assumed to set in at all points within the region of integration before  $\ell$  reaches  $\ell_0$ .

This case can be handled in the same way as the  $q$  integration in A.1. The only minor difference occurs, when proving the analogon to Lemma 1. We will use Lemma 1' proved at the end of this section.

The set of all elements in the  $k_z, k_\perp$  plane such that  $\alpha_q(k_z, k_\perp, \infty) = 0$ ,  $S := \{(k_z, k_\perp) | \alpha_q(k_z, k_\perp, \infty) = 0\}$ , is a regular one dimensional compact manifold.

We have:

$$\begin{aligned}
 & \int_B d^3 k \alpha_{k,q}(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \\
 &= \int_B d^3 k \alpha_q(k, \ell) |M_q|^2 e^{-2 \int_0^\ell (\alpha_q(k, \ell'))^2 d\ell'} \\
 &= 2\pi |M_q|^2 \int_{B^2} dk_z dk_\perp \quad k_\perp \alpha_q(k_z, k_\perp, \ell) e^{-2 \int_0^\ell (\alpha_q(k_z, k_\perp, \ell'))^2 d\ell'} \\
 &= 2\pi |M_q|^2 \int_{|\alpha_q(k_z, k_\perp, \infty)| \leq \delta} dk_z dk_\perp \quad k_\perp \alpha_q(k_z, k_\perp, \ell) e^{-2 \int_0^\ell (\alpha_q(k_z, k_\perp, \ell'))^2 d\ell'} \\
 &= 2\pi |M_q|^2 \int_{|\alpha_q(k_z, k_\perp, \infty)| \leq \delta} dk_z dk_\perp \quad k_\perp \left( \alpha_q(k_z, k_\perp, \infty) + \frac{d_q(k_z, k_\perp)}{2\sqrt{\ell}} \right) \\
 &\quad \times \exp -2\ell \left( \alpha_q(k_z, k_\perp, \infty) + \frac{d_q(k_z, k_\perp)}{\sqrt{\ell}} \right)^2 \ell^{-\frac{1}{2}} d_q^2(k_z, k_\perp) \\
 &\quad \times \exp -2[\alpha_q(k_z, k_\perp, \ell^*)^2 - \alpha_q(k_z, k_\perp, \infty)^2] \ell_0 \\
 &\quad \times \exp \left( 2(2d_q(k_z, k_\perp) \alpha_q(k_z, k_\perp, \infty) \sqrt{\ell_0} + d_q^2(k_z, k_\perp) \frac{1}{4} \ln \ell_0) \right) \quad \exp 2d_q^2(k_z, k_\perp)
 \end{aligned} \tag{A.36}$$

From second to third line we introduced cylindrical coordinates with  $q$  beeing the  $z$ -axis and performed the integration over the angle; from third to fourth line we used

Lemma 2; from fourth to fifth line we wrote  $\alpha_q(k_z, k_\perp, \ell)$  explicitly in the asymptotic regime as defined in (A.3).

We now use Lemma 1' to again introduce a transformation of variables  $(k_z, k_\perp) \rightarrow (t, u)$ . Once again we find 1 for the jacobian determinant. For our integral we then have, rewriting  $k_\perp = \tilde{k}(t, u)$ :

$$\begin{aligned}
 & 2\pi |M_q|^2 \int_{|\alpha_q(t, u, \infty)| \leq \delta} dt du \left( \alpha_q(t, u, \infty) + \frac{d_q(t, u)}{2\sqrt{\ell}} \right) \tilde{k}(t, u) \\
 & \times \exp -2\ell \left( \alpha_q(t, u, \infty) + \frac{d_q(t, u)}{\sqrt{\ell}} \right)^2 \ell^{-\frac{1}{2}d_q^2(t, u)} \\
 & \times \exp -2[\alpha_q(t, u, \ell^*)^2 - \alpha_q(t, u, \infty)^2] \ell_0 \\
 & \times \exp \left( 2(2d_q(t, u)\alpha_q(t, u, \infty)\sqrt{\ell_0} + d_q^2(t, u)\frac{1}{4} \ln \ell_0) \right) \exp 2d_q^2(t, u)
 \end{aligned} \tag{A.37}$$

We now have an integral of exactly the same form as before and, hence, continue analogously:

$$\begin{aligned}
 & 2\pi |M_q|^2 \int_B dt \int_{z \leq \delta} dz \frac{1}{\frac{\partial \alpha}{\partial u}|_{t, u(t, z)}} \left( z + \frac{d_q(t, z)}{2\sqrt{\ell}} \right) \tilde{k}(t, z) \\
 & \times \exp -2\ell \left( z + \frac{d_q(t, z)}{\sqrt{\ell}} \right)^2 \ell^{-\frac{1}{2}d_q^2(t, z)} \\
 & \times \exp -2[\alpha_q(t, z, \ell^*)^2 - z^2] \ell_0 \\
 & \times \exp \left( 2(2d_q(t, z)z\sqrt{\ell_0} + d_q^2(t, z)\frac{1}{4} \ln \ell_0) \right) \exp 2d_q^2(t, z)
 \end{aligned} \tag{A.38}$$

$$\begin{aligned}
 &= 2\pi |M_q|^2 \int_B dt \int_{(z' - \frac{d_q(t,z)}{\sqrt{\ell}}) \leq \delta} dz' \frac{1}{1 + \frac{1}{\sqrt{\ell}} \frac{\partial d_q}{\partial z} |_{t,z(t,z')}} \frac{1}{\frac{\partial \alpha}{\partial u} |_{t,u(t,z' - \frac{d_q(t,z)}{\sqrt{\ell}})}} \\
 &\quad \times (z' - \frac{d_q(t,z' - \frac{d_q(t,z)}{\sqrt{\ell}})}{2\sqrt{\ell}}) \tilde{k}(t, z' - \frac{d_q(t,z)}{\sqrt{\ell}}) \\
 &\quad \times \exp -2\ell(z')^2 \ell^{-\frac{1}{2}d_q^2(t, z' - \frac{d_q(t,z)}{\sqrt{\ell}})} \\
 &\quad \times \exp -2[\alpha_q(t, z' - \frac{d_q(t,z)}{\sqrt{\ell}}, \ell^*)^2 - (z' - \frac{d_q(t,z)}{\sqrt{\ell}})^2] \ell_0 \\
 &\quad \times \exp 2(2d_q(t, z' - \frac{d_q(t,z)}{\sqrt{\ell}})(z' - \frac{d_q(t,z)}{\sqrt{\ell}})\sqrt{\ell_0} + d_q^2(t, z' - \frac{d_q(t,z)}{\sqrt{\ell}})\frac{1}{4} \ln \ell_0) \exp 2d_q^2(t, z' - \frac{d_q(t,z)}{\sqrt{\ell}})
 \end{aligned} \tag{A.39}$$

$$\begin{aligned}
 &= -\frac{1}{\sqrt{2}} \pi^{\frac{3}{2}} |M_q|^2 \frac{1}{\ell} \int_{B^3} d^3k \delta(\alpha_q(k)) \left[ d_q(k) \tilde{k} \ell^{-\frac{1}{2}d_q^2(k)} \right. \\
 &\quad \left. \times \exp -2[\alpha_q(k, \ell^*)^2] \ell_0 \exp (d_q^2(k)\frac{1}{2} \ln \ell_0) \exp 2d_q^2(k) \right]
 \end{aligned} \tag{A.40}$$

$$\begin{aligned}
 &= -\frac{1}{\sqrt{2}} \pi^{\frac{3}{2}} |M_q|^2 \frac{1}{\ell} \int_B dt \frac{1}{\frac{\partial \alpha}{\partial u} |_{t,u(t,z')}} (d_q(t)) \tilde{k}(t) \ell^{-\frac{1}{2}d_q^2(t)} \\
 &\quad \times \exp -2[\alpha_q(t, \ell^*)^2] \ell_0 \exp (d_q^2(t)\frac{1}{2} \ln \ell_0) \exp 2d_q^2(t)
 \end{aligned} \tag{A.41}$$

This proves the second part of (A.2)

In order to justify the above Lemma 1' remains to be proven:

### Lemma 1'

The set of all elements in the  $k_z, k_\perp$  plane such that  $\alpha_q(k_z, k_\perp, \infty) = 0$ ,  $S := \{(k_z, k_\perp) | \alpha_q(k_z, k_\perp, \infty) = 0\}$ , is a regular one dimensional compact manifold.

Proof:

a) The set  $S := \{(k_z, k_\perp) | \alpha_q(k_z, k_\perp, \infty) = 0\}$  is compact: As  $B^2$  is bounded,  $S$  is bounded as well. As  $B^2$  is closed and  $\alpha_q(k_z, k_\perp, \infty)$  is continuous,  $S$  is closed. Thus  $S$  is compact.

b) We show, that  $S$  does not contain isolated points. A point in  $S$  can only be isolated, if it is a local minimum or maximum of  $\alpha_k(p, q, \infty)$ ,

i.e.  $\frac{\partial \alpha_q(k_z, k_\perp, \infty)}{\partial k_z} = \frac{\partial \alpha_q(k_z, k_\perp, \infty)}{\partial k_\perp} = 0$ . This can be proved very easily using the theorem on implicit functions.

To investigate, whether isolated points exist, we take a look at the first derivatives: As  $\frac{\partial \alpha_q}{\partial k_z} = \frac{\partial \epsilon}{\partial x} \Big|_{x=\sqrt{(k_z+q)^2+k_\perp^2}} \times \frac{k_z+q}{\sqrt{(k_z+q)^2+k_\perp^2}} - \frac{\partial \epsilon}{\partial x} \Big|_{x=\sqrt{k_z^2+k_\perp^2}} \times \frac{k_z}{\sqrt{k_z^2+k_\perp^2}}$ .

It is easily seen, that:  $\alpha_q(k_z, k_\perp, \ell) > 0 \ \forall \ell, k_z > 0$ . Further  $\frac{\partial \alpha}{\partial k_z} > 0$  and  $-q < k_z < 0$  (as  $\frac{\partial \epsilon}{\partial x} > 0$ ). We now use our assumption, that  $\frac{\partial \epsilon}{\partial x}$  is strictly monotonously increasing

and the fact, that:  $\left| \frac{k_z+q}{\sqrt{(k_z+q)^2+k_\perp^2}} \right| > \left| \frac{k_z}{\sqrt{k_z^2+k_\perp^2}} \right| \ k_z < -q$ . This immediately shows:

$\frac{\partial \alpha_q(k_z, k_\perp, \infty)}{\partial k_z} > 0$  and  $k_z < -q$ . Thus  $S$  cannot contain isolated points.

As  $\alpha_q(k_z, k_\perp^0, \infty)$  is strictly monotonously increasing with  $k_z \ \forall k_z < 0$  and thus in the entire region, where  $\alpha_q(k_z, k_\perp, \infty) \leq 0$ ,  $S$  is connected (unless cut into parts by the region of integration).

The above proves Lemma 1'

## B. A more refined asymptotic Behaviour

### B.1. General Remarks and Outline

In this appendix we investigate the equations (4.12)-(4.14), using a different Ansatz for the flow of the electronic energies in the asymptotic regime. The asymptotic behaviour for the flow of the phonons remains unchanged in leading order. We have shown, that a  $\frac{1}{\ell^\gamma}$  behaviour in the asymptotic is only possible as long as  $\gamma = \frac{1}{2}$ , we have not investigated a  $\frac{1}{\ell^{\frac{1}{2} \ln \ell}}$  behaviour. This we do here.

We set:

$$\omega(\ell) = \omega(\infty) + \frac{1}{2\sqrt{\ell + \ell_0(q)}} + \frac{e(q)}{2\sqrt{\ell + \ell_1(q)} \ln(\ell + \ell_1(q))} \quad (\text{B.1})$$

and

$$\epsilon(\ell) = \epsilon(\infty) + \frac{e(k)}{2\sqrt{\ell + \ell_\epsilon(k)} \ln(\ell + \ell_\epsilon(k))} \quad (\text{B.2})$$

as before we have:

$$\begin{aligned} \alpha_{k,q}(\ell) &:= \epsilon_{k+q}(\ell) - \epsilon_k(\ell) + \omega_q(\ell) \\ &= \alpha_{k,q}(\infty) + \frac{e(k+q)}{2\sqrt{\ell + \ell_\epsilon(k+q)} \ln(\ell + \ell_\epsilon(k+q))} - \frac{e(k)}{2\sqrt{\ell + \ell_\epsilon(k)} \ln(\ell + \ell_\epsilon(k))} \\ &\quad + \frac{1}{2\sqrt{\ell + \ell_0(q)}} + \frac{e(q)}{2\sqrt{\ell + \ell_1(q)} \ln(\ell + \ell_1(q))} \end{aligned} \quad (\text{B.3})$$

we will continue to use  $\alpha := \alpha_{k,q} := \alpha_{k,q}(\infty)$ ;  $\alpha(\ell) := \alpha_{k,q}(\ell)$

For the electrons the decay under the  $\ell$  induced flow is now only given by a  $\frac{1}{\sqrt{\ell} \ln \ell}$  term. We also introduce one additional change in this chapter. Up to now we have always assumed, that the asymptotic behaviour has already set in, we only have the case, where  $\ell \gg \ell_0$ , and we have always assumed  $\ell + \ell_i$  to equal  $\ell$ . Off course, this is right for the left hand side of (4.12-4.14), as we are investigating the asymptotic case. But on the right hand side the integrals contain regions, where  $\ell_0$  is larger than  $\ell$ . To deal with this problem we assume the above asymptotic behaviour for  $\ell > \ell_i$ . For the case  $\ell < \ell_1(q)$  we assume the phononic energies to be given by:

$$\omega(\ell) = \omega(\infty) + \frac{1}{2\sqrt{\ell + \ell_0(q)}} + \frac{e_q}{2\sqrt{2\ell_1(q)} \ln(2\ell_1(q))} \quad (\text{B.4})$$

For  $\ell < \ell_\epsilon$  the electronic energies are given by:

$$\epsilon(\ell) = \epsilon(\infty) + \frac{e(k)}{2\sqrt{2\ell_\epsilon(k)} \ln(2\ell_\epsilon(k))} \quad (\text{B.5})$$

Using this Ansatz for the asymptotic behaviour and its onset the integrals for the calculation of  $\frac{d\omega_q}{d\ell}$  und  $\frac{d\epsilon_k}{d\ell}$  are given by three parts:

$$\begin{aligned} \frac{d\omega_q}{d\ell} &= \int_{\substack{\ell > \ell_\epsilon(k) \\ \ell > \ell_\epsilon(k+q)}} \alpha(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} (n_{k+q} - n_k) d^3 k \\ &+ \int_{\substack{\ell < \ell_\epsilon(k) \\ \ell > \ell_\epsilon(k+q)}} \alpha(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} (n_{k+q} - n_k) d^3 k \\ &+ \int_{\substack{\ell > \ell_\epsilon(k), \\ \ell < \ell_\epsilon(k+q)}} \alpha(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} (n_{k+q} - n_k) d^3 k \end{aligned} \quad (\text{B.6})$$

and for the electrons:

$$\begin{aligned} \frac{d\epsilon_k}{d\ell} &= \int_{\substack{\ell > \ell_1(q) \\ \ell > \ell_\epsilon(k+q)}} \alpha(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} (1 - n_{k+q}) d^3 q \\ &+ \int_{\substack{\ell_0 < \ell < \ell_1(q), \\ \ell > \ell_\epsilon(k+q)}} \alpha(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} (1 - n_{k+q}) d^3 q \\ &+ \int_{\substack{\ell > \ell_0(q) \\ \ell < \ell_\epsilon(k+q)}} \alpha(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} (1 - n_{k+q}) d^3 q \end{aligned} \quad (\text{B.7})$$

The idea is, of course, to choose the expression of the left hand side to be of its asymptotic form. As the integrand for the integrals governing the derivatives of the phononic and electronic energies is the same, we evaluate this integrand in the next section. We then calculate the derivatives of the phononic and electronic energies in the two subsequent sections. It finally turns out, that a self-consistent solution for constant  $e(k)$  and  $e(q)$  cannot be found<sup>1</sup>. Nevertheless, using the asymptotic behaviour only for  $\ell$  larger than a certain threshold and an even faster decay of the electronic energies makes the effort worthwhile.

## B.2. The Integrand

For the calculation of  $\frac{d\omega}{d\ell}$  and  $\frac{d\epsilon}{d\ell}$  (see (B.6) and (B.7)) the integrand is given by:

$$\alpha_{k,q}(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \quad (\text{B.8})$$

---

<sup>1</sup>This does not, however, show, that no solution with varying  $e(k)$  and  $e(q)$  exists.

For the evaluation we use Ansatz (B.1) and (B.2). Later we put  $e(q) = 0$ ,  $e(k) = 0$  or  $e(k+q) = 0$  to also evaluate those regions of the integrals, where the asymptotic behaviour has not yet set in for all terms contained in  $\alpha$ .

In a first step we now calculate the integral:

$$\begin{aligned}
 & \int_0^\ell \alpha(\ell')^2 d\ell' \\
 &= \int_0^\ell \left( \alpha(\infty) + \frac{1}{2\sqrt{\ell' + \ell_0(q)}} + \frac{e(k+q)}{2\sqrt{\ell' + \ell_\epsilon(k+q)} \ln(\ell' + \ell_\epsilon(k+q))} \right. \\
 & \quad \left. - \frac{e(k)}{2\sqrt{\ell' + \ell_\epsilon(k)} \ln(\ell' + \ell_\epsilon(k))} + \frac{e(q)}{2\sqrt{\ell' + \ell_1(q)} \ln(\ell' + \ell_1(q))} \right)^2 d\ell' \\
 &= \alpha^2 \ell + 2\alpha \sqrt{\ell + \ell_0(q)} - 2\alpha \sqrt{\ell_0(q)} + 2e(k+q)\alpha \frac{\sqrt{\ell + \ell_\epsilon(k+q)}}{\ln(\ell + \ell_\epsilon(k+q))} - 2e(k+q)\alpha \frac{\sqrt{\ell_\epsilon(k+q)}}{\ln(\ell_\epsilon(k+q))} \\
 & \quad - 2e_k \alpha \frac{\sqrt{\ell + \ell_\epsilon(k)}}{\ln(\ell + \ell_\epsilon(k))} + 2e_k \alpha \frac{\sqrt{\ell_\epsilon(k)}}{\ln(\ell_\epsilon(k))} + 2e_q \alpha \frac{\sqrt{\ell + \ell_1(q)}}{\ln(\ell + \ell_1(q))} - 2e_q \alpha \frac{\sqrt{\ell_1(q)}}{\ln(\ell_1(q))} \\
 & \quad + \frac{1}{4} \ln(\ell + \ell_0(q)) - \frac{1}{4} \ln \ell_0(q) + \frac{e(k+q)}{2} \ln \ln(\ell + \ell_\epsilon(k+q)) - \frac{e(k+q)}{2} \ln \ln(\ell_\epsilon(k+q)) \\
 & \quad - \frac{e_k}{2} \ln \ln(\ell + \ell_\epsilon(k)) + \frac{e_k}{2} \ln \ln(\ell_\epsilon(k)) + \frac{e_q}{2} \ln \ln(\ell + \ell_1(q)) - \frac{e_q}{2} \ln \ln(\ell_1(q)) \\
 & \quad + \frac{\sum_{i,j} e_i e_j}{4} \left( \frac{1}{\ln \ell + \ell_?} - \frac{1}{\ln \ell_?} \right)
 \end{aligned} \tag{B.9}$$

where we neglected terms of the order of:  $\int \frac{1}{\sqrt{\ell' + \ell_i} \ln^2(\ell' + \ell_i)} d\ell'$ . In the last line we understand the  $e_i$  to equal our  $e(q)$ ,  $-e(k)$  or  $e(k+q)$ . For convenience we will also use  $\ell_i$  instead of  $\ell_1$  or  $\ell_\epsilon$ . The constant  $\ell_?$  depends on  $\ell_0$  and  $\ell_\epsilon$ . As  $e^{\frac{1}{\ln \ell}} \rightarrow 1$  as  $\ell \rightarrow \infty$  we will subsequently drop this term altogether.

We also approximated:

$$\int \frac{1}{\sqrt{\ell' + \ell_0(q)} \sqrt{\ell' + \ell_\epsilon(k)} \ln(\ell' + \ell_\epsilon(k))} d\ell' \quad \text{by} \quad \ln \ln(\ell + \ell_\epsilon(k)) \tag{B.10}$$

Because we discuss equation (B.9) in the asymptotic region only, we can set:  $\frac{1}{\sqrt{\ell + \ell_i}} = \frac{1}{\sqrt{\ell}}$  and  $\frac{1}{\sqrt{\ell + \ell_j} \ln(\ell + \ell_j)} = \frac{1}{\sqrt{\ell} \ln \ell}$  and the expression simplifies to:

$$\begin{aligned}
& \ell \left[ \alpha + \frac{1}{\sqrt{\ell}} + \frac{(e(k+q)-e(k)+e(q))}{\sqrt{\ell} \ln(\ell)} \right]^2 - 1 \\
& - 2\alpha \left[ \sqrt{2\ell_0} + e(k+q) \frac{\sqrt{\ell_\epsilon(k+q)}}{\ln(\ell_\epsilon(k+q))} - e_k \frac{\sqrt{\ell_\epsilon(k)}}{\ln(\ell_\epsilon(k))} + e_q \frac{\sqrt{\ell_\epsilon(q)}}{\ln(\ell_\epsilon(q))} \right] \\
& + \frac{1}{4} \ln(\ell) - \frac{1}{4} \ln(\ell_0(q)) \\
& + \frac{(e(k+q)-e(k)+e(q))}{2} \ln \ln(\ell) - \frac{e(k+q)}{2} \ln \ln(\ell_\epsilon(k+q)) + \frac{e_k}{2} \ln \ln(\ell_\epsilon(k)) - \frac{e_q}{2} \ln \ln(\ell_1(q))
\end{aligned} \tag{B.11}$$

As the integrals in (B.6) and (B.7) are confined to  $\alpha \approx 0$  the second line is of no importance and can be omitted, and we find for the integrand:

$$\begin{aligned}
& \alpha(\ell) |M_q|^2 e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} \\
& = \tilde{c}^2 q \left( \alpha + \frac{1}{2\sqrt{\ell}} + \frac{e(k+q)-e(k)+e(q)}{2\sqrt{\ell} \ln(\ell)} \right) \\
& \times e^{-2\ell \left[ \alpha + \frac{1}{\sqrt{\ell}} + \frac{(e(k+q)-e(k)+e(q))}{\sqrt{\ell} \ln(\ell)} \right]^2} e^2 \frac{1}{\sqrt{\ell}} \sqrt{\ell_0(q)} \\
& \times (\ln(\ell))^{\frac{(e(k+q)-e(k)+e(q))}{2}} (\ln(\ell_\epsilon(k+q)))^{-e_{k+q}} (\ln(\ell_\epsilon(k)))^{e_k} (\ln(\ell_1(q)))^{-e_q}
\end{aligned} \tag{B.12}$$

where we used again:  $M_q = \tilde{c}\sqrt{q}$   
later we will also use:  $\omega_q(0) = cq$ .

### B.3. Derivative of the phononic energies

We now calculate the derivative of the phonon-energies:

We use:  $\frac{1}{\sqrt{\ell+\ell_0}} = \frac{1}{\sqrt{\ell}}$  we set  $e_{k,q} = -e(k+q) - e(k) + e(q)$

then we have:

$$\begin{aligned}
\frac{d\omega_q(\ell)}{d\ell} &= 2 \sum_k |M_{k,q}(\ell)|^2 \alpha_{k,q}(\ell) (n_{k+q} - n_k) \\
&= 2\Gamma \int_{B_z} |M_q(\ell)|^2 \alpha_{k,q}(\ell) e^{-2 \int_0^\ell \alpha^2(\ell') d\ell'} (n_{k+q} - n_k)
\end{aligned}$$

As in previous chapters we integrate over the azimuthal variable and as argued in section 5.1 the region of integration given by:  $n_{k+q} = 0, n_k = 1$  contributes only an



exponentially decaying term to the asymptotic behaviour and is omitted as before, the relevant region of integration is the same as in section 5.3.1. We use the result to write the integral as:

$$4\pi\Gamma\tilde{c}^2qe^2\int_{k_f}^{\sqrt{(k_f)^2-2k_zq-q^2}}dkk\int_{-k}^{-\frac{q}{2}}dk_z\left(\alpha-\frac{1}{2\sqrt{\ell}}-\frac{e_{k,q}}{2\sqrt{\ell}\ln(\ell)}\right)e^{-2l\alpha^2} \quad (\text{B.13})$$

$$\frac{1}{\sqrt{\ell}}\sqrt{\ell_0}(\ln(\ell))^{-(e(k+q)-e(k)+e(q))}(\ln\ell_\epsilon(k+q))^{e(k+q)}(\ln\ell_\epsilon(k))^{-e_k}(\ln\ell_1(q))^{e_q}$$

N.B. As discussed above the value of  $e_{k+q}$  and  $e_k$  depend on the corresponding region of integration in (B.6). E.g. for  $\ell_\epsilon(k) > \ell$  we set  $e_k = 0$ , as  $\ell_\epsilon(\ell)$  does not contain a  $\ell$ -dependent term for  $\ell < \ell_\epsilon(k)$ .

We change variables:  $\alpha = \frac{k_zq}{m} + \frac{q^2}{2m} + cq$

$$4\pi\Gamma\tilde{c}^2me^2\int_{k_f}^{\sqrt{(k_f)^2-2k_z(\alpha)q-q^2}}dkk\int_{-\frac{kq}{m}+\frac{q^2}{2m}+cq}^{cq}d\alpha\left(\alpha-\frac{1}{2\sqrt{\ell}}-\frac{e_{k,q}}{2\sqrt{\ell}\ln(\ell)}\right)e^{-2l\alpha^2} \quad (\text{B.14})$$

$$\frac{1}{\sqrt{\ell}}\sqrt{\ell_0}(\ln(\ell))^{-(e(k+q)-e(k)+e(q))}(\ln\ell_\epsilon(k+q))^{e(k+q)}(\ln\ell_\epsilon(k))^{-e_k}(\ln\ell_1(q))^{e_q}$$

As  $\frac{k_fq}{m} \gg \frac{q^2}{2m} + cq$ , we can use the same arguments as in Chapter 4 and in Appendix A to proceed:

$$2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell}\int_{k_f}^{\sqrt{(k_f)^2-2k_z(0)q-q^2}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)\left(-\frac{1}{2\sqrt{\ell}}-\frac{e_{k,q}}{2\sqrt{\ell}\ln(\ell)}\right) \quad (\text{B.15})$$

$$\times\sqrt{\ell_0}(\ln(\ell))^{-(e(k+q)-e(k)+e(q))}(\ln\ell_\epsilon(k+q))^{e(k+q)}(\ln\ell_\epsilon(k))^{-e_k}(\ln\ell_1(q))^{+e_q}$$

It has to be discussed, whether we can simply drop the constant term added to  $\alpha$  in equations (B.4) and (B.5) when performing the calculation of our integral above. In chapter 5 (except for section 5.5) we have always replaced  $\alpha_{k,q}(\infty)$  by  $\alpha_{k,q}(\infty)$ , when evaluating our  $\delta(\alpha)$  function. This is justified as we do not expect the form of  $\alpha$  to change significantly under the  $\ell$ -dependent transformation. Hence, to proceed the same way for this calculation remains justified.

We have:  $|k+q| = \sqrt{k^2+q^2+2k_zq} = \sqrt{k^2-2mcq+2m\alpha}$ ; for  $\alpha = 0$ , this turns out to be  $\sqrt{k^2-2mcq}$ .

For the constants we now make the following Ansatz for mathematical convenience:

$$\begin{aligned} \ell_0(q) &= \frac{D-1}{q^2} & \ell_1(q) &= e^{\frac{1}{q^2}} & \ell_\epsilon(k) &= e^{\frac{1}{(k-k_f)^2}} \\ e(k) &= \frac{1}{2} \text{sgn}(k - k_f); & (e_k = 0, \quad \ell_\epsilon(k) > \ell; & \quad e_{k+q} = 0, \quad \ell_\epsilon(k+q) > \ell); \\ e(q) &= 1 \end{aligned} \tag{B.16}$$

Now the three parts of our integral are given by:

$$2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{D-1}{q}\frac{1}{\ell}\int_{k_f+\frac{1}{\sqrt{\ln\ell}}}^{\sqrt{(k_f-\frac{1}{\sqrt{\ln\ell}})^2+2mcq}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)\left(-\frac{1}{2\sqrt{\ell}}\right) \tag{B.17}$$

$$\begin{aligned} &\times\left(\frac{1}{(|k+q|-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{(k-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{q^2}\right) \\ &+2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell}\frac{D-1}{q}\int_{k_f}^{k_f+\frac{1}{\sqrt{\ln\ell}}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)\left(-\frac{1}{2\sqrt{\ell}}-\frac{\frac{1}{2}}{2\sqrt{\ell}\ln(\ell)}\right) \end{aligned} \tag{B.18}$$

$$\begin{aligned} &\times(\ln(\ell))^{-\frac{1}{2}}\left(\frac{1}{(|k+q|-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{q^2}\right) \\ &+2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell}\frac{D-1}{q}\int_{\sqrt{(k_f-\frac{1}{\sqrt{\ln\ell}})^2+2mcq}}^{\sqrt{k_f^2+2mcq}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)\left(-\frac{1}{2\sqrt{\ell}}-\frac{\frac{1}{2}}{2\sqrt{\ell}\ln(\ell)}\right) \end{aligned} \tag{B.19}$$

$$\times(\ln(\ell))^{-\frac{1}{2}}\left(\frac{1}{(k-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{q^2}\right)$$

We present the calculation of these three terms in the following three subsections.

### B.3.1. Region of integration: $|k+q| < k_f - \frac{1}{\sqrt{\ln\ell}}$ and $k > k_f + \frac{1}{\sqrt{\ln\ell}}$

We now start by evaluating the first of the integrals given above in line (B.17):

$$\begin{aligned} &-\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q^3} \\ &\times\int_{k_f+\frac{1}{\sqrt{\ln\ell}}}^{\sqrt{(k_f-\frac{1}{\sqrt{\ln\ell}})^2+2mcq}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)||k+q|-k_f|(k-k_f) \end{aligned} \tag{B.20}$$

$$\begin{aligned}
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D_{-1}}{q^3} \\
 &\times \int_{k_f+\frac{1}{\sqrt{\ln \ell}}}^{\sqrt{(k_f-\frac{1}{\sqrt{\ln \ell}})^2+2mcq}} dk k |\sqrt{k^2-2mcq}-k_f|(k-k_f)
 \end{aligned} \tag{B.21}$$

As  $q$  is small compared to  $k_f$  and  $k \approx k_f$  we have:  $\sqrt{k^2+2mcq} \approx k + \frac{mcq}{k} \approx k + \frac{mcq}{k_f}$  :

$$\begin{aligned}
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D_{-1}}{q^3}k_f \\
 &\times \int_{\frac{1}{\sqrt{\ln \ell}}}^{(-\frac{1}{\sqrt{\ln \ell}})+\frac{mcq}{k_f}} d\Delta k \left| \left( \Delta k - \frac{mcq}{k_f} \right) \right| (\Delta k) \\
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D_{-1}}{q^3}k_f \\
 &\times \left| \left[ \frac{1}{3}(\Delta k)^3 - \frac{1}{2}\frac{mcq}{k_f}(\Delta k)^2 \right]_{\frac{1}{\sqrt{\ln \ell}}}^{(-\frac{1}{\sqrt{\ln \ell}})+\frac{mcq}{k_f}} \right| \\
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D_{-1}}{q^3}k_f \\
 &\times \left( +\frac{1}{6}\left(\frac{mc}{k_f}\right)^3q^3 - \frac{mc}{k_f}\frac{q}{\ln \ell} + \frac{2}{3}\frac{1}{\sqrt{\ln \ell}^3} \right) \\
 &= -\frac{\sqrt{2}}{6}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2\frac{m^4c^3}{k_f^2}e^2D_{-1}\frac{1}{\ell^{\frac{3}{2}}} + hoT
 \end{aligned} \tag{B.22}$$

As in (5.37) we can again choose  $D_{-1}$  such that  $b(q) = 1 + h.o.T.$ . But now  $D_{-1}$  contains another factor of  $\frac{k_f^2}{m^2c^2}$  i.e. without the counter factor  $D_{-1}$  the above is a lot smaller than the expression in (5.36).

**B.3.2. Region of integration:**  $k_f \leq k < k_f + \frac{1}{\sqrt{\ln \ell}}$

For the second integral (B.18) we have:

$$\begin{aligned}
& 2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{D-1}{q}}}\int_{k_f}^{k_f+\frac{1}{\sqrt{\ln \ell}}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)\left(-\frac{1}{2\sqrt{\ell}}-\frac{\frac{1}{2}}{2\sqrt{\ell}\ln(\ell)}\right) \\
& \quad \times (\ln(\ell))^{-\frac{1}{2}}\left(\frac{1}{(|k+q|-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{q^2}\right) \\
& = -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}\left(\frac{1}{\ln \ell}+\frac{\frac{1}{2}}{\sqrt{\ln \ell}^3}\right) \\
& \quad \times \int_{k_f}^{k_f+\frac{1}{\sqrt{\ln \ell}}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)||k+q|-k_f| \\
& = -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}\left(\frac{1}{\ln \ell}+\frac{\frac{1}{2}}{\sqrt{\ln \ell}^3}\right) \\
& \quad \times \int_{k_f}^{k_f+\frac{1}{\sqrt{\ln \ell}}}dkk\left|\left(\sqrt{k^2-2mcq}-k_f\right)\right|
\end{aligned} \tag{B.23}$$

We once again use the approximations  $\sqrt{k^2+2mcq} \approx k + \frac{mcq}{k} \approx k + \frac{mcq}{k_f}$  and  $k \approx k_f$ .

$$\begin{aligned}
& -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}k_f\left(\frac{1}{\ln \ell}+\frac{\frac{1}{2}}{\sqrt{\ln \ell}^3}\right) \\
& \quad \times \int_{k_f}^{k_f+\frac{1}{\sqrt{\ln \ell}}}dk\left|\left(k-\frac{mcq}{k_f}-k_f\right)\right| \\
& = -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}k_f\left(\frac{1}{\ln \ell}+\frac{\frac{1}{2}}{\sqrt{\ln \ell}^3}\right) \\
& \quad \times \int_0^{\frac{1}{\sqrt{\ln \ell}}}d\Delta k\left|\left(\Delta k-\frac{mcq}{k_f}\right)\right| \\
& = -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}k_f\left(\frac{1}{\ln \ell}+\frac{\frac{1}{2}}{\sqrt{\ln \ell}^3}\right) \\
& \quad \times \left|\left[\frac{1}{2}(\Delta k)^2-\frac{mcq}{k_f}\Delta k\right]_0^{\frac{1}{\sqrt{\ln \ell}}}\right|
\end{aligned} \tag{B.24}$$

$$\begin{aligned}
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}k_f\left(\frac{1}{\ln\ell}+\frac{\frac{1}{2}}{\sqrt{\ln\ell}^3}\right)\left(-\frac{1}{2}\frac{1}{\ln\ell}+\frac{mcq}{k_f}\frac{1}{\sqrt{\ln\ell}}\right) \\
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}k_f\frac{mcq}{k_f}\left(\frac{1}{\ln\ell}-\frac{1}{2}\frac{1}{\sqrt{\ln\ell}^3}\right)+h.o.T.
 \end{aligned} \tag{B.25}$$

### B.3.3. Region of integration: $k_f \geq |k+q| > k_f - \frac{1}{\sqrt{\ln\ell}}$

By straightforward calculation or by arguments of symmetry it is immediately seen, that this integral (B.19) yields the same result as the previous one.

$$\begin{aligned}
 &+2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}\int\frac{\sqrt{k_f^2+2mcq}}{\sqrt{(k_f-\frac{1}{\sqrt{\ln\ell}})^2+2mcq}}dkk\int_{-\infty}^{\infty}d\alpha\delta(\alpha)\left(-\frac{1}{2\sqrt{\ell}}-\frac{\frac{1}{2}}{2\sqrt{\ell}\ln(\ell)}\right) \\
 &\quad \times (\ln(\ell))^{-\frac{1}{2}}\left(\frac{1}{(k-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{q^2}\right)^1 \\
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q}k_f\frac{mcq}{k_f}\left(\frac{1}{\ln\ell}-\frac{1}{2}\frac{1}{\sqrt{\ln\ell}^3}\right)
 \end{aligned} \tag{B.26}$$

### B.3.4. The derivative of the Phononic Energies

Combining the three results from above we have:

$$\begin{aligned}
 &\frac{d\omega_q(\ell)}{d\ell} \\
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q^3}k_f \\
 &\quad \times \left(+\frac{1}{6}\left(\frac{mc}{k_f}\right)^3q^3-\frac{mc}{k_f}\frac{q}{\ln\ell}+\frac{2}{3}\frac{1}{\sqrt{\ln\ell}^3}\right) \\
 &\quad -2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}\frac{D-1}{q^3}k_f\left(\frac{mcq}{k_f}\frac{q}{\ln\ell}-\frac{1}{2}\frac{1}{\sqrt{\ln\ell}^3}\right) \\
 &= -\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2me^2\frac{1}{\ell^{\frac{3}{2}}}D_{-1}k_f\left(\frac{1}{6}\left(\frac{mc}{k_f}\right)^3\right. \\
 &\quad \left.+\frac{mcq}{k_f}\frac{1}{q^2}\frac{1}{\ln\ell}-\frac{1}{3}\frac{1}{q^3}\frac{1}{\sqrt{\ln\ell}^3}\right)
 \end{aligned} \tag{B.27}$$

### B.3.5. Discussion

This result is interesting, as  $D_{-1}$  can still be chosen such that the leading term of (B.27) equals  $\frac{-1}{4\sqrt{\ell}}$ , the right leading term for the flow of the phononic energies. It is not suprising that the terms of higher logarithmic order in  $\ell$  are not given correctly, the onset of the asymptotic behaviour at  $\ell = \ell_\epsilon$  is a very crude assumption. In addition the  $\ell_\epsilon$  can still be refined by using additional constants, i.e.:

$$\ell_\epsilon(k) = \text{const}_1 e^{\frac{\text{const}_2}{(k-k_f)^2}}.$$

## B.4. Change of the Electronic Energies

Using the results of B.2, we now calculate the derivatives of the electronic energies, in exactly the same way as for the phonons:

$$\begin{aligned} & \frac{d\epsilon_k(\ell)}{d\ell} \\ &= -2\Gamma \int \alpha_{k,q}(\ell) |M_q(\ell)|^2 (1 - n_{k+q}) d^3q \\ &= -2\Gamma \tilde{c}^2 \int q \alpha_{k,q}(\ell) e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} (1 - n_{k+q}) d^3q \\ &= -4\pi\Gamma \tilde{c}^2 \left( \int_0^{k-k_f} dq q^2 \int_{-q}^q dq_z + \int_{k-k_f}^D dq q^2 \int_{\frac{k_f^2 - k^2 - q^2}{2k}}^q dq_z \right) \left( \alpha_{k,q}(\ell) e^{-2 \int_0^\ell \alpha_{k,q}^2(\ell') d\ell'} \right) \end{aligned} \quad (\text{B.28})$$

where D is the upper limit of the Brillouin zone. Inserting (B.12), gives:

$$\begin{aligned} \frac{d\epsilon_k(\ell)}{d\ell} &= -4\pi\Gamma \tilde{c}^2 e^2 \left( \int_0^{k-k_f} dq q^2 \int_{-q}^q dq_z + \int_{k-k_f}^D dq q^2 \int_{\frac{k_f^2 - k^2 - q^2}{2k}}^q dq_z \right) \\ &\quad \times \left[ \left( \alpha - \frac{1}{2\sqrt{\ell}} - \frac{e_{k,q}}{2\sqrt{\ell} \ln(\ell)} \right) e^{-2l\alpha^2} \right. \\ &\quad \left. \times \frac{1}{\sqrt{\ell}} \sqrt{\ell_0} (\ln(\ell))^{-e_{k,q}} (\ln \ell_\epsilon(k+q))^{e(k+q)} (\ln \ell_\epsilon(k))^{-e_k} (\ln \ell_1(q))^{e_q} \right] \end{aligned} \quad (\text{B.29})$$

where  $e_{k,q} = e(k+q) - e(k) + e(q)$  and, as before,  $\alpha := \alpha_{k,q}(\infty)$ .

We set:

$\tilde{C} := 4\pi\Gamma\tilde{c}^2e^2$  and

$$\tilde{I} := \frac{1}{\sqrt{\ell}} \sqrt{\ell_0} (\ln(\ell))^{-e_{k,q}} (\ln \ell_\epsilon(k+q))^{e(k+q)} (\ln \ell_\epsilon(k))^{-e_k} (\ln \ell_1(q))^{e_q} \quad (\text{B.30})$$

And we change variables:  $q_z \rightarrow \alpha = \frac{k}{m}q_z + \frac{q^2}{2m} + cq$  to write the two terms as:

$$\begin{aligned} -\tilde{C} & \left( \int_0^{k-k_f} dq q^2 \int_{-\frac{k}{m}q + \frac{q^2}{2m} + cq}^{\frac{k}{m}q + \frac{q^2}{2m} + cq} d\alpha \frac{m}{k} + \int_{k-k_f}^D dq q^2 \int_{\frac{\frac{k}{m}q + \frac{q^2}{2m} + cq}{\frac{k_f^2 - k^2 + 2cmq}{2m}}} d\alpha \frac{m}{k} \right) \\ & \times \left( \alpha - \frac{1}{2\sqrt{\ell}} - \frac{e_{k,q}}{2\sqrt{\ell}\ln(\ell)} \right) \tilde{I} e^{-2l\alpha^2} \end{aligned} \quad (\text{B.31})$$

For all those values of  $q$ , for which the  $\alpha$ -integral does not contain  $\alpha = 0$ , the latter integral is going to decay exponentially. For the first term of (B.31) we have:

$-\frac{k}{m}q + \frac{q^2}{2m} + cq < 0$  and  $\frac{k}{m}q + \frac{q^2}{2m} + cq > 0$ , but for the second part we can drop those parts of the  $q$ -integral, where:  $\frac{k_f^2 - k^2 + 2cmq}{2m} > 0$ , i.e.  $q = \frac{k^2 - k_f^2}{2mc}$  is effectively the upper boundary to the  $q$ -integral.

For smaller  $q$  the range of the  $\alpha$ -integration contains  $\alpha = 0$  and hence any negative lower and positive upper boundary can be used for  $\ell$  large enough.

$$-\tilde{C} \int_0^{\frac{k^2 - k_f^2}{2mc}} dq q^2 \int_{-\frac{k}{m}q + \frac{q^2}{2m} + cq}^{\frac{k}{m}q + \frac{q^2}{2m} + cq} d\alpha \frac{m}{k} \left( \alpha - \frac{1}{2\sqrt{\ell}} - \frac{e_{k,q}}{2\sqrt{\ell}\ln(\ell)} \right) \tilde{I} e^{-2l\alpha^2} \quad (\text{B.32})$$

For increasing  $\ell$  we have:

I.e.  $\int_{-b}^a f(\alpha, q, \ell) \sqrt{\ell} e^{-2l\alpha^2} d\alpha = \frac{\sqrt{\pi}}{\sqrt{2}} \int_{-\infty}^{\infty} f(\alpha, q, \ell) \delta(\alpha) d\alpha$ , with  $a, b$  arbitrary positive real numbers.

Thus:

$$\frac{d\epsilon_k(\ell)}{d\ell} = -2\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{1}{\sqrt{\ell}} \int_0^{\frac{k^2 - k_f^2}{2mc}} q^2 \frac{m}{k} \left( -\frac{1}{2\sqrt{\ell}} - \frac{e_{k,q}}{2\sqrt{\ell}\ln(\ell)} \right) \tilde{I} dq \quad (\text{B.33})$$

We insert the values of the  $e(k), e(q), \ell_\epsilon$  as given in (B.16) in the equation given above

and the integral splits into three parts:

$$\begin{aligned}
\frac{d\epsilon_k(\ell)}{d\ell} &= \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{1}{\ell^{\frac{3}{2}}}\int_{\frac{1}{\sqrt{\ln\ell}}}^{\frac{k^2-(k_f+\frac{1}{\sqrt{\ln\ell}})^2}{2mc}}q^2\frac{m}{k}\left(1+\frac{1}{\ln\ell}\right) \\
&\times\frac{D-1}{q}(\ln\ell)^{-1}\left(\frac{1}{(|k+q|-k_f)^2}\right)^{\frac{1}{2}}\left(\frac{1}{(k-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{q^2}\right)dq \\
&+\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{1}{\ell^{\frac{3}{2}}}\int_0^{\frac{1}{\sqrt{\ln\ell}}}q^2\frac{m}{k}\frac{D-1}{q}\left(\frac{1}{(|k+q|-k_f)^2}\right)^{\frac{1}{2}}\left(\frac{1}{(k-k_f)^2}\right)^{-\frac{1}{2}}dq \\
&+\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{1}{\ell^{\frac{3}{2}}}\int_{\frac{k^2-k_f^2}{2mc}}^{\frac{k^2-(k_f+\frac{1}{\sqrt{\ln\ell}})^2}{2mc}}q^2\frac{m}{k}\left(1+\frac{1}{\ln\ell}\right) \\
&\times\frac{D-1}{q}(\ln\ell)^{-\frac{1}{2}}\left(\frac{1}{(k-k_f)^2}\right)^{-\frac{1}{2}}\left(\frac{1}{q^2}\right)dq
\end{aligned} \tag{B.34}$$

For the second term in this equation we have assumed that the  $\frac{\text{const}}{\sqrt{\ell+\ell_0}}$  term in the asymptotic behaviour is present for all values of  $q$  in (B.4). This is possible without any error in the leading order as the only part where  $\ell_0 > \ell$  is given by:  $q < \frac{1}{\sqrt{\ell}}$  and leads to an integral bounded like:  $\int_0^{\frac{1}{\sqrt{\ell}}}$ . This leads to terms decaying faster than  $\frac{\text{const}}{\ell^2}$ . We now continue our evaluations for the three parts of this equation separately:

#### B.4.1. Central Region of Integration

We can write the first of the three terms as:

$$\begin{aligned}
&\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}(k-k_f)\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\left(1+\frac{1}{\ln\ell}\right) \\
&\times\int_{\frac{1}{\sqrt{\ln\ell}}}^{\frac{k^2-(k_f+\frac{1}{\sqrt{\ln\ell}})^2}{2mc}}dq\frac{1}{q}\left|\frac{1}{(|k+q|-k_f)}\right|
\end{aligned} \tag{B.35}$$

For  $\alpha = 0$ , we have  $|k+q| = \sqrt{k^2 - 2mcq} \approx k + \frac{mcq}{k} \approx k - \frac{mcq}{k_f}$ , as both  $k - k_f$  and  $q$  are small. This yields:



$$\begin{aligned}
 & \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}(k-k_f)\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\left(1+\frac{1}{\ln\ell}\right) \\
 & \times \int_{\frac{1}{\sqrt{\ln\ell}}}^{\frac{k^2-(k_f+\frac{1}{\sqrt{\ln\ell}})^2}{2mc}} dq \frac{1}{q} \left( \frac{1}{(k-k_f-\frac{mcq}{k_f})} \right) \\
 & = \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}(k-k_f)\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\left(1+\frac{1}{\ln\ell}\right) \\
 & \times \frac{1}{k-k_f} \int_{\frac{1}{\sqrt{\ln\ell}}}^{\frac{k^2-(k_f+\frac{1}{\sqrt{\ln\ell}})^2}{2mc}} dq \left( \frac{1}{q} + \frac{\frac{mc}{k_f}}{(k-k_f-\frac{mcq}{k_f})} \right)
 \end{aligned} \tag{B.36}$$

We simplify the upper boundary of the integral ( $(k+k_f) \approx 2k_f$  and  $\frac{1}{\ln\ell} \ll \frac{1}{\sqrt{\ln\ell}}$ ) and find:

$$\begin{aligned}
 & = \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\left(1+\frac{1}{\ln\ell}\right) \int_{\frac{1}{\sqrt{\ln\ell}}}^{\frac{k_f}{mc}(k-k_f-\frac{1}{\sqrt{\ln\ell}})} dq \left( \frac{1}{q} + \frac{\frac{mc}{k_f}}{(k-k_f-\frac{mcq}{k_f})} \right) \\
 & = \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\left(1+\frac{1}{\ln\ell}\right) \left[ \ln q - \ln(k-k_f-\frac{mcq}{k_f}) \right]_{\frac{1}{\sqrt{\ln\ell}}}^{\frac{k_f}{mc}(k-k_f-\frac{1}{\sqrt{\ln\ell}})} \\
 & = \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\left(1+\frac{1}{\ln\ell}\right) \left[ \ln\left(\frac{k_f}{mc}(k-k_f)\right) - 2\ln\frac{1}{\sqrt{\ln\ell}} + \ln(k-k_f) \right] \\
 & = \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\left(1+\frac{1}{\ln\ell}\right) \left[ \ln\left(\frac{k_f}{mc}\right) + 2\ln(k-k_f) + \ln\ln\ell \right]
 \end{aligned} \tag{B.37}$$

$$= \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln\ell} \ln\ln\ell + h.o.T. \tag{B.38}$$

This results shows that the solution is not truly self consistent. However, the  $\ln\ln\ell$  term can be canceled by inserting an additional term of the form  $\frac{e_q}{2\sqrt{\ell}\ln\ell\ln\ln\ell}$  and  $\frac{e_k}{2\sqrt{\ell}\ln\ell\ln\ln\ell}$  into the asymptotic behaviour of the phononic and electronic energies in equations (B.1) and (B.2).

**B.4.2. Region of integration:**  $0 < q < \frac{1}{\sqrt{\ln \ell}}$

The second part of (B.34) is given by:

$$\begin{aligned}
 & \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}}\left(1+\frac{1}{\ln(\ell)}\right)\int_0^{\frac{1}{\sqrt{\ln \ell}}}dq q\left(\frac{1}{(|k+q|-k_f)^2}\right)^{\frac{1}{2}}\left(\frac{1}{(k-k_f)^2}\right)^{-\frac{1}{2}} \\
 &= \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}(k-k_f)\frac{1}{\ell^{\frac{3}{2}}}\left(1+\frac{1}{\ln(\ell)}\right)\int_0^{\frac{1}{\sqrt{\ln \ell}}}dq q\left(\frac{1}{(|k+q|-k_f)}\right) \quad (\text{B.39}) \\
 &= \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}(k-k_f)\frac{1}{\ell^{\frac{3}{2}}}\left(1+\frac{1}{\ln(\ell)}\right)\int_0^{\frac{1}{\sqrt{\ln \ell}}}dq q\left(\frac{1}{(k-k_f-\frac{mcq}{k_f})}\right)
 \end{aligned}$$

Using  $\frac{1}{k-k_f-\frac{mc}{k_f\sqrt{\ln \ell}}} = \frac{1}{k-k_f}$  the integral is readily evaluated and we find:

$$\frac{1}{\sqrt{2}}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}}\frac{1}{\ln \ell} + h.o.T. \quad (\text{B.40})$$

**B.4.3. Region of integration:**  $k_f < |k+q| < k_f + \frac{1}{\sqrt{\ln \ell}}$

Now only the third part of (B.34) remains to be calculated:

$$\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}(k-k_f)\frac{1}{\ell^{\frac{3}{2}}\sqrt{\ln \ell}}\left(1+\frac{1}{\ln(\ell)}\right)\int_{\frac{k^2-k_f^2}{2mc}}^{\frac{k^2-k_f^2}{2mc}+\frac{1}{\sqrt{\ln \ell}}}dq \frac{1}{q} \quad (\text{B.41})$$

We use  $\int_{\frac{k_f}{mc}(k-k_f-\frac{1}{\sqrt{\ln \ell}})}^{\frac{k_f}{mc}(k-k_f)}\frac{1}{q}dq = \ln(\frac{k_f}{mc}(k-k_f)) - \ln(\frac{k_f}{mc}(k-k_f) - \frac{1}{\sqrt{\ln \ell}})$   
 $= -\ln\left(1 - \frac{1}{(k-k_f)\sqrt{\ln \ell}}\right) \approx \frac{1}{(k-k_f)\sqrt{\ln \ell}}$  to find:

$$\sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln \ell} + h.o.T. \quad (\text{B.42})$$

**B.4.4. The Derivative of the Electronic Energies**

We have thus found - taking into account the effects of the terms:  $\frac{e_q}{2\sqrt{\ell}\ln \ell \ln \ln \ell}$  and  $\frac{e_k}{2\sqrt{\ell}\ln \ell \ln \ln \ell}$  in (B.1) and (B.2)-:

$$\frac{d\epsilon_k(\ell)}{d\ell}$$

$$\begin{aligned}
 &= \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln\ell} \\
 &+ \sqrt{2}\pi^{\frac{3}{2}}\Gamma\tilde{c}^2e^2\frac{m}{k}D_{-1}\frac{1}{\ell^{\frac{3}{2}}\ln\ell}\frac{1}{\ln\ln\ell}\left[\left(\ln\left(\frac{k_f}{mc}\right) + 2\ln(k - k_f)\right) + \frac{3}{4}\right] \quad (\text{B.43}) \\
 &+ h.o.T.
 \end{aligned}$$

#### B.4.5. Discussion

In this appendix we have investigated an Ansatz for  $\epsilon_k(\ell)$  and  $\omega_q(\ell)$  given in (B.1) and (B.2). The Ansatz could very well be refined by inserting constants into the values of  $\ell_1$  and  $\ell_\epsilon$  in (B.16), e.g.  $\ell_1 = \text{const}_1 e^{\frac{\text{const}_2}{q^2}}$ . Even if these constants are set to equal one we do refind the right leading order when evaluating the derivatives of the electronic and phononic flow according to (B.6) and (B.7).

Still the following contradiction appears: In (B.16) we have assumed  $e(k)$  to be positive for  $k > k_f$ . That means  $e(k)$  has the same sign, as the leading  $\frac{\text{const}}{\sqrt{\ell+\ell_0}}$  term in (B.1). But, comparing the results in (B.27) and the first line of (B.16) shows, that this cannot be fulfilled.



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